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ACT GAR643S/A

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L29 SCR 72
L30 STR
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L32 STR
L33 113 SEA FILE=REGISTRY SUB=L31 SSS FUL L32

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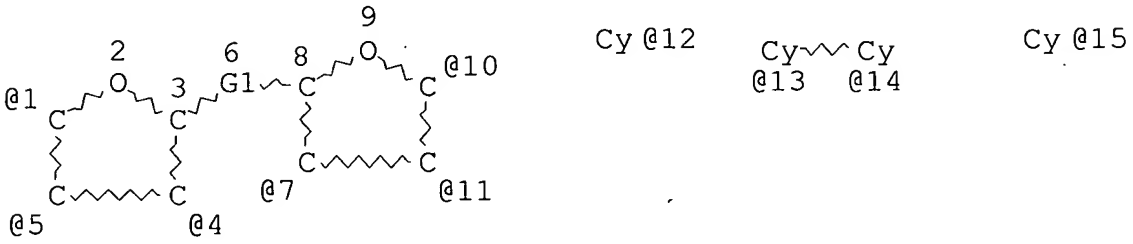

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GRAPH ATTRIBUTES:
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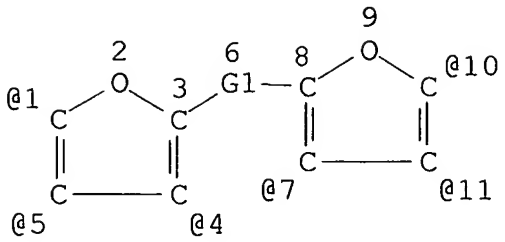

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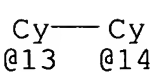

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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L33 113 SEA FILE=REGISTRY SUB=L31 SSS FUL L32
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L36 35 SEA FILE=HCA ABB=ON PLU=ON L34 NOT L35

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=> d l36 1-35 ibib abs hitstr hitind

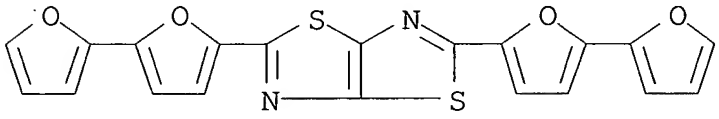
L36 ANSWER 1 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 141:430217 HCA
TITLE: Characterization and field-effect transistor performance of heterocyclic oligomers containing a thiazolothiazole unit
AUTHOR(S): Ando, Shinji; Nishida, Junichi; Fujiwara, Eiichi; Tada, Hirokazu; Inoue, Youji; Tokito, Shizuo; Yamashita, Yoshiro
CORPORATE SOURCE: Department of Electronic Chemistry, Interdisciplinary Graduate School of Science and

Engineering, Tokyo Institute of Technology, Yokohama, 226-8502, Japan
SOURCE: Chemistry Letters (2004), 33(9), 1170-1171
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Novel mixed five-membered heterocyclic (furan, thiophene, and thiazole) oligomers containing a thiazolothiazole ring system were studied as active materials of organic field-effect transistors (OFETs). The field-effect moblities of 10-4-10-3 cm2/Vs were obtained for the furyl derivs. and their FET performances as p-type semiconductors are presented as the 1st examples of FET behavior of oligomers including furan rings.

IT **794589-24-5**
(elec. and optical and thermal properties of organic field-effect transistors based on heterocyclic oligomers containing a thiazolothiazole unit)

RN 794589-24-5 HCA
CN INDEX NAME NOT YET ASSIGNED



CC 76-3 (Electric Phenomena)
Section cross-reference(s): 22, 28

IT 110-00-9D, Furan, derivative 110-02-1D, Thiophene, derivative 251-56-9D,
Thiazolo[5,4-d]thiazole, derivative 288-47-1D, Thiazole, derivative
741292-15-9 794589-21-2 794589-22-3 794589-23-4
794589-24-5
(elec. and optical and thermal properties of organic field-effect transistors based on heterocyclic oligomers containing a thiazolothiazole unit)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 140:391683 HCA
TITLE: DFT study of conjugated biheterocyclic oligomers exhibiting a very low HOMO-LUMO energy gap
AUTHOR(S): Ammar Aouchiche, Hafida; Djennane, Sema; Boucekkine, Abdou
CORPORATE SOURCE: Laboratoire de Chimie Theorique, Faculte de

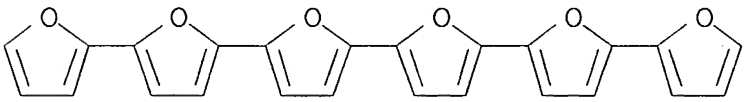
Chimie, Algiers, 16111, Algeria
SOURCE: Synthetic Metals (2004), 140(2-3), 127-133
CODEN: SYMEDZ; ISSN: 0379-6779
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB D. functional theory (DFT) was applied to study the structure and electronic properties of oligomers based on bithiophene bridged by a sp2 carbon substituted by a chalcogen atom (O, S, Se and Te), and their poly(bifuran) and poly(bipyrrole) analogs. The important reduction of the energy gap which is observed for the whole series of biheterocyclic compds., when going down the chalcogen group, is explained on the basis of an orbital interaction anal. Bithiophene polymers bridged by a selenium or a tellurium substituted carbon atom are expected to exhibit low energy band gap.

IT **174895-49-9**
(DFT study of effect of chalcogen bridge on electronic structure of conjugated bi-heterocyclic oligomers exhibiting very low HOMO-LUMO energy gap)

RN 174895-49-9 HCA

CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2'''''-Sexifuran (9CI) (CA INDEX NAME)



CC 36-5 (Physical Properties of Synthetic High Polymers)
Section cross-reference(s): 65, 76

IT 5632-29-1, 2,2':5',2'':5'',2'''-Quaterthiophene 5905-00-0, 2,2'-Bifuran 10087-64-6, 2,2'-Bipyrrole 25796-77-4, Cyclopenta[2,1-b:3,4-b']dithiophen-7-one 56902-08-0, Bithiophene 80421-31-4, 2,2':5',2'':5'',2'''-Quaterfuran 86450-98-8, 2,2':5',2'':5'',2'''-Quater-1H-pyrrole 88493-55-4 108664-05-7 **174895-49-9** 241809-58-5 241809-65-4 241809-66-5 241809-68-7, 4H-Cyclopenta[2,1-b:3,4-b']difuran-4-one 241809-69-8 685870-55-7 685870-56-8 685870-57-9 685870-58-0 685870-59-1 685870-60-4
(DFT study of effect of chalcogen bridge on electronic structure of conjugated bi-heterocyclic oligomers exhibiting very low HOMO-LUMO energy gap)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 3 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 139:261645 HCA

TITLE: Production method of metallocene compounds useful for olefin polymerization catalysts and production method of polyolefins therewith

INVENTOR(S): Nakano, Masato; Shiota, Tsutomu; Moriyama, Ryohei; Yamazaki, Hiroshi

PATENT ASSIGNEE(S): Chisso Corp., Japan; Chisso Petrochemical Corporation

SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

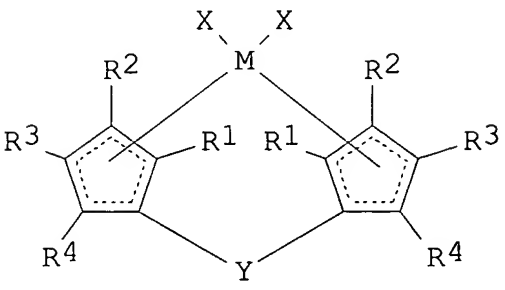
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003261587	A2	20030919	JP 2002-60342	20020306

PRIORITY APPLN. INFO.: JP 2002-60342 20020306

OTHER SOURCE(S): MARPAT 139:261645

GI



I

AB Title metallocene compds. are represented by the general formula I, where R1 = independently H, C1-6 alkyl, halogen or Si containing C1-6 hydrocarbyl, (halogen containing) C6-16 aryl, R2 = independently substituted 2-furyl or substituted 2-thienyl, R3-4 = independently H, C1-6 alkyl, halogen or Si containing C1-6 hydrocarbyl, alkyl, (halogen containing) C6-16 aryl, (substituted) 2-furyl, or (substituted)

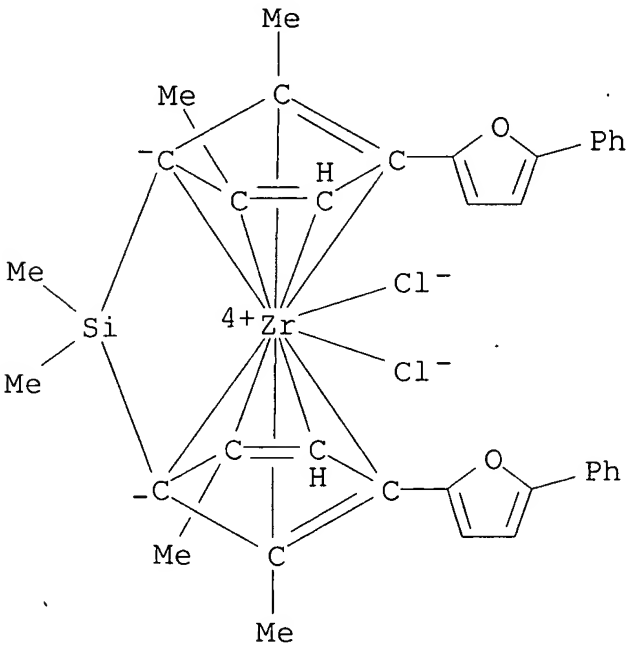
2-thienyl, M = Ti, Zr, or Hf, X = halogen or C1-6 alkyl, and Y = ethylene, methylene, C1-6 alkyl containing dialkylsilylene, dialkylgermirene, tetraalkylethylene, dialkylmethylene, C6-16 aryl containing diarylsilylene or diarylgermirene, C1-6 alkyl and C6-16 aryl containing alkylarylsilylene or alkylarylgermirene. The compds. are used as polymerization catalysts for olefins to give polyolefins with high stereoregularity in high catalyst activities. Thus, propylene was polymerized in the presence of MMAO 3A and racemic dimethylsilylenebis[3-(2'-(5'-phenyl)furyl)-2,5-dimethylcyclopentadienyl]zirconium dichloride obtained from 2-phenylfuran, 3,5-dimethylcyclopentene-1-one, dimethyldichlorosilane, and zirconium tetrachloride to give a polypropylene with polymerization activity 80 kg-polymer/mmol-Zr-h, MFR 9.2 g/10 min, Mw/Mn 1.80, and m.p. 151.4°.

IT **601468-67-1P**

(preparation of metallocene compds. useful for olefin polymerization catalysts)

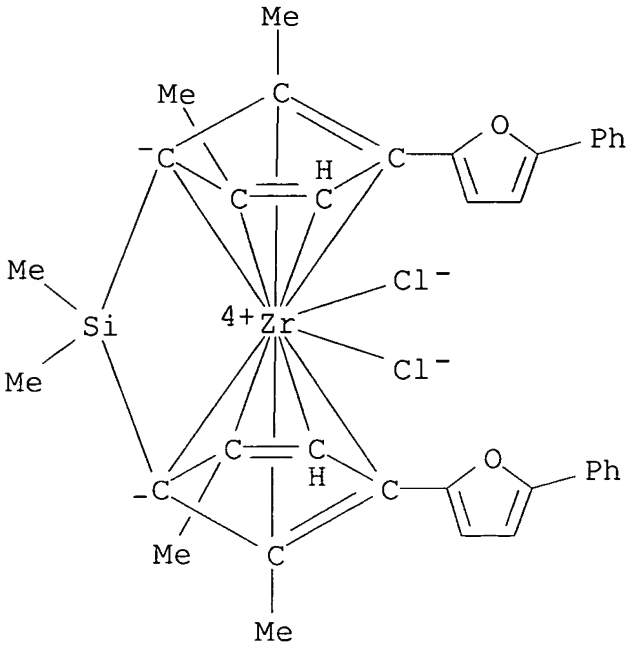
RN 601468-67-1 HCA

CN Zirconium, dichloro[rel-(1R,1'R)-(dimethylsilylene)bis[(1,2,3,4,5-η)-2,5-dimethyl-3-(5-phenyl-2-furanyl)-2,4-cyclopentadien-1-ylidene]]- (9CI) (CA INDEX NAME)



IT **601472-45-1P**

(preparation of metallocene compds. useful for olefin polymerization
catalysts)
RN 601472-45-1 HCA
CN Zirconium, dichloro[(dimethylsilylene)bis[(1,2,3,4,5-η)-2,5-dimethyl-3-(5-phenyl-2-furanyl)-2,4-cyclopentadien-1-ylidene]]-(9CI) (CA INDEX NAME)



IC ICM C07F017-00
ICS C07F007-00; C07F007-08; C08F004-658; C08F010-00
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67
IT **601468-67-1P** 601468-72-8P
(preparation of metallocene compds. useful for olefin polymerization
catalysts)
IT 601468-71-7P **601472-45-1P**
(preparation of metallocene compds. useful for olefin polymerization
catalysts)

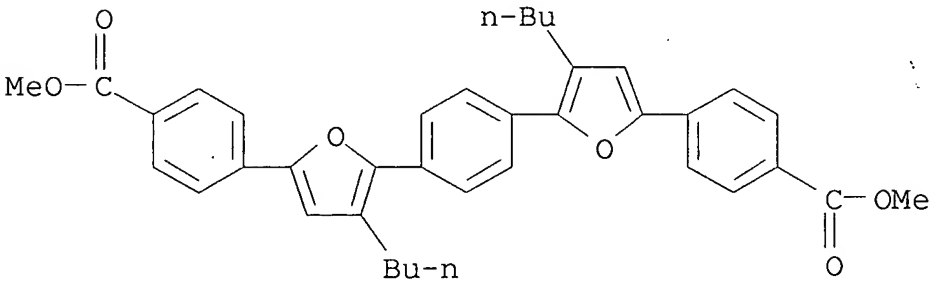
L36 ANSWER 4 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 138:337903 HCA
TITLE: Bidirectional iterative synthesis of alternating benzene-furan oligomers towards molecular wires
AUTHOR(S): Lee, Chin-Fa; Liu, Ching-Yuan; Song, Hua-Can; Luo, Shr-Jie; Tseng, Jui-Chang; Tso, Hsi-Hua;

Luh, Tien-Yau
CORPORATE SOURCE: Institute of Chemistry, Academia Sinica, Taipei, 115, Taiwan
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (23), 2824-2825
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:337903

AB Reaction of propargylic dithioacetal with BuLi gives the sulfur-substituted allenyllithium which is allowed to react with a dialdehyde to yield the corresponding alternating benzene-furan oligoaryls (A). Functional group transformation converts the ester groups in A to dialdehyde which can be used for the synthesis of higher homologues towards mol. wires. A combination of this furan annulation, Heck reaction and Sonogashira coupling leads to a variety of benzene-furan-alkene/alkyne conjugated oligomers of precise length.

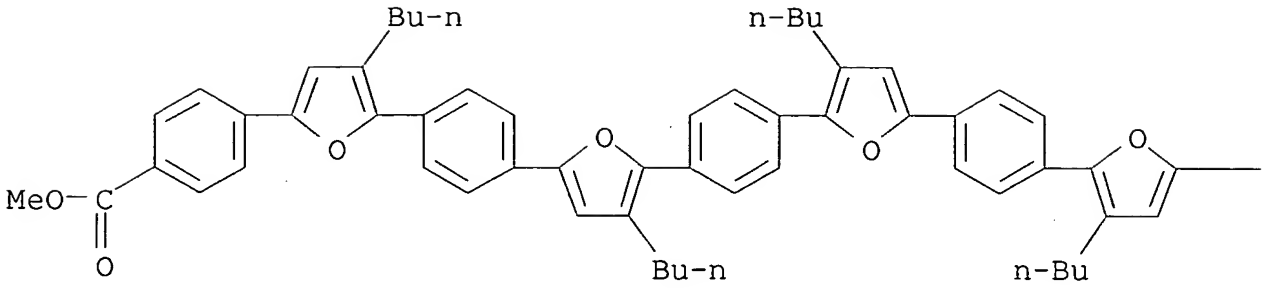
IT **515139-35-2P 515139-37-4P 515139-44-3P 515139-45-4P**
(preparation of alternating benzene-furan oligomers via reaction of propargylic dithioacetal with butyllithium followed by reaction with aldehydes and photophys. and electrochem. of products useful for mol. wire applications)

RN 515139-35-2 HCA
CN Benzoic acid, 4,4'-[1,4-phenylenebis(4-butyl-5,2-furandiyl)]bis-, dimethyl ester (9CI) (CA INDEX NAME)



RN 515139-37-4 HCA
CN Benzoic acid, 4,4'-[1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylene(4-butyl-5,2-furandiyl)]]bis-, dimethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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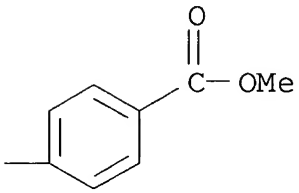
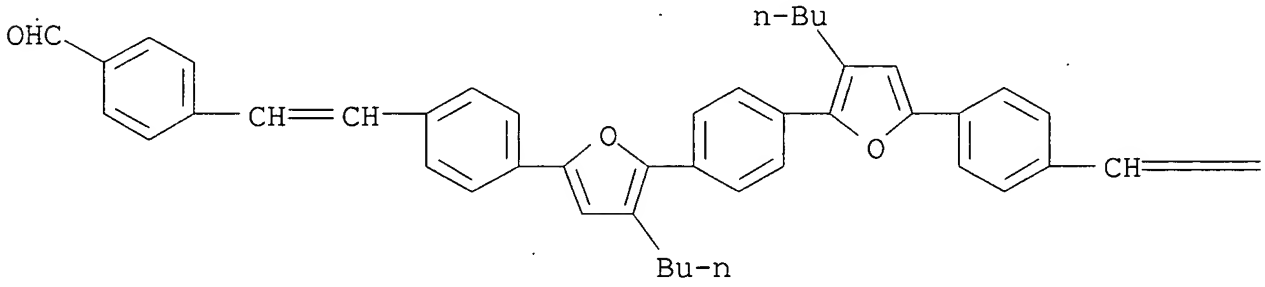


RN 515139-44-3 HCA
CN Benzaldehyde, 4,4'-[1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylene-2,1-ethenediyl]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



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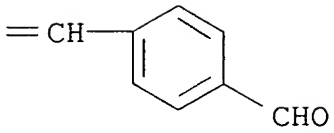
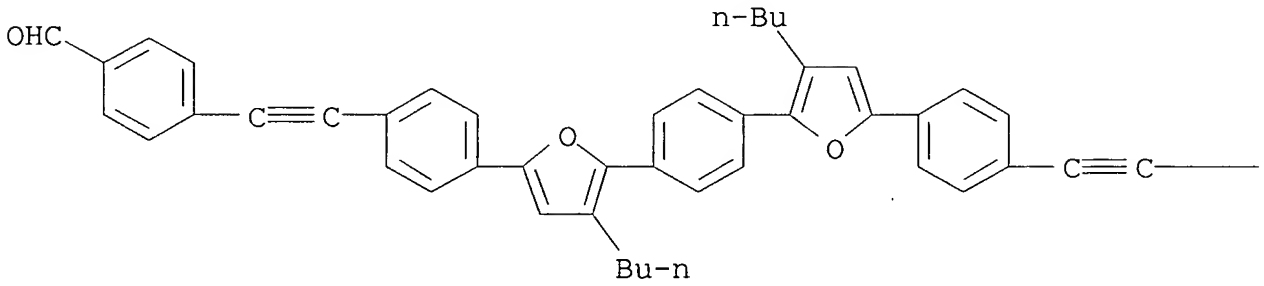


RN 515139-45-4 HCA
CN Benzaldehyde, 4,4'-[1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylene-2,1-ethynediyl]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



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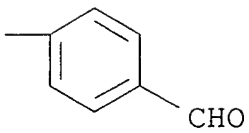
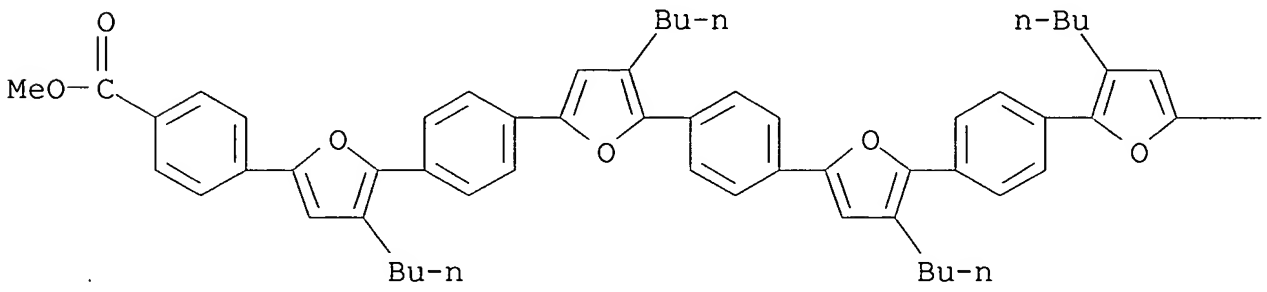


IT **515139-39-6P 515139-43-2P 515139-46-5P**
515139-47-6P 515139-48-7P
(preparation of alternating benzene-furan oligomers via reaction of propargylic dithioacetal with butyllithium followed by reaction with aldehydes and photophys. and electrochem. of products useful for mol. wire applications)
RN 515139-39-6 HCA

CN Benzoic acid, 4,4'-[1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylene(4-butyl-5,2-furandiyl)-4,1-phenylene(4-butyl-5,2-furandiyl)]]bis-, dimethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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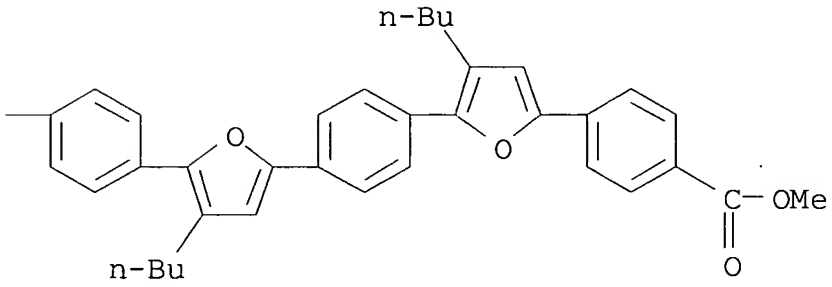
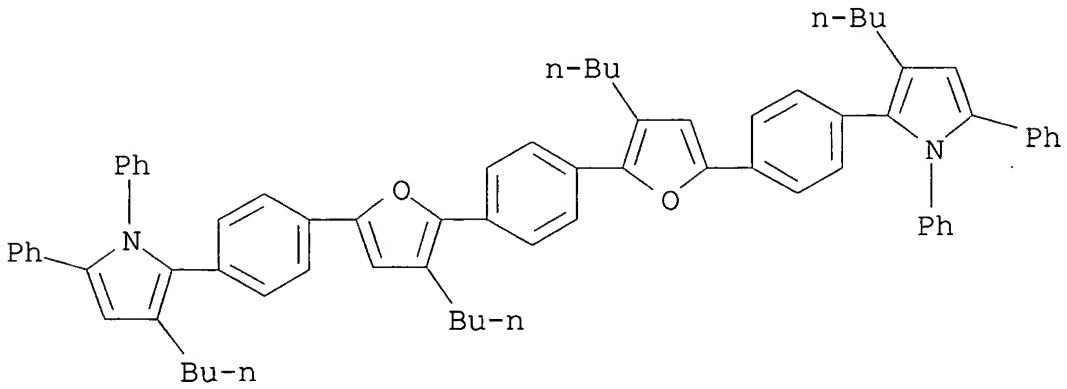


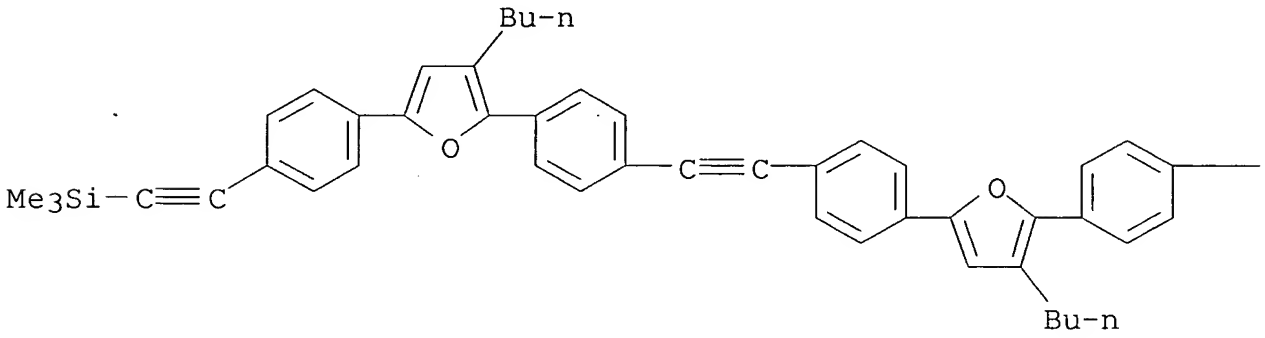
RN 515139-43-2 HCA

CN 1H-Pyrrole, 2,2'-[1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylene]]bis[3-butyl-1,5-diphenyl- (9CI) (CA INDEX NAME)



RN 515139-46-5 HCA
CN Silane, [1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylene-2,1-ethynediyl-4,1-phenylene(4-butyl-5,2-furandiyl)-4,1-phenylene-2,1-ethynediyl]]bis[trimethyl- (9CI) (CA INDEX NAME)

PAGE 1-A



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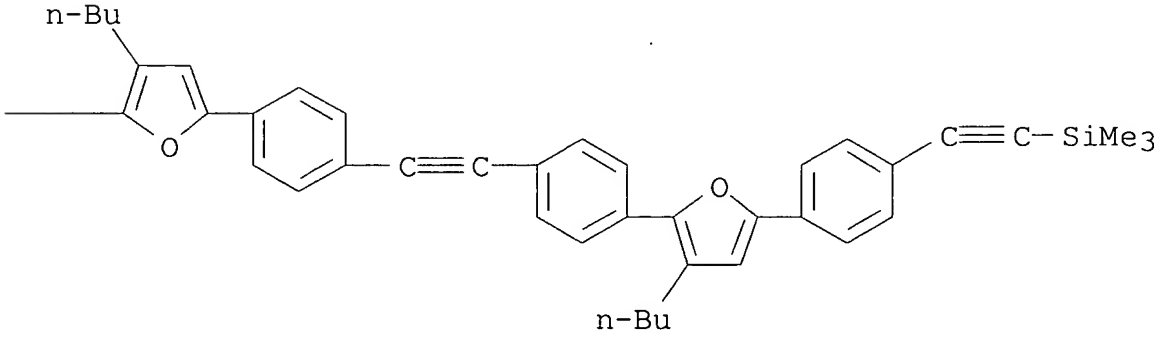
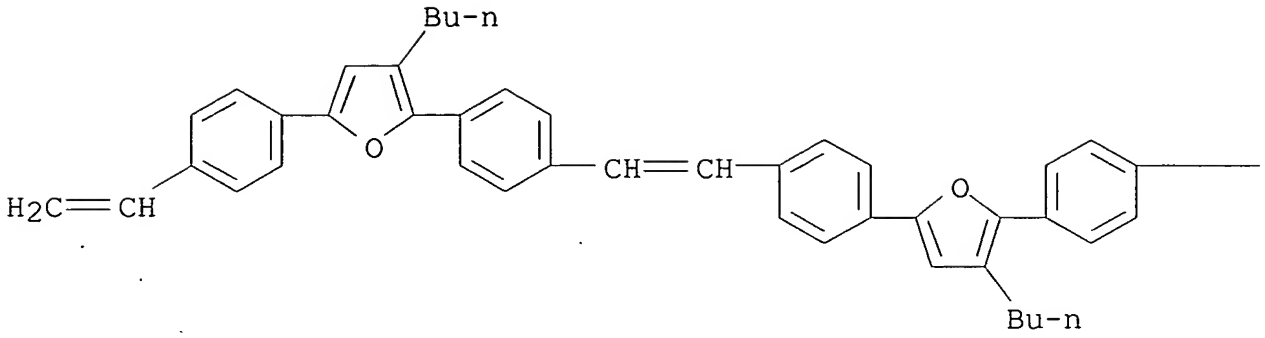


RN 515139-47-6 HCA
CN Furan, 2,2'-(1,4-phenylene)bis[3-butyl-5-[4-[2-[4-[3-butyl-5-(4-ethenylphenyl)-2-furanyl]phenyl]ethenyl]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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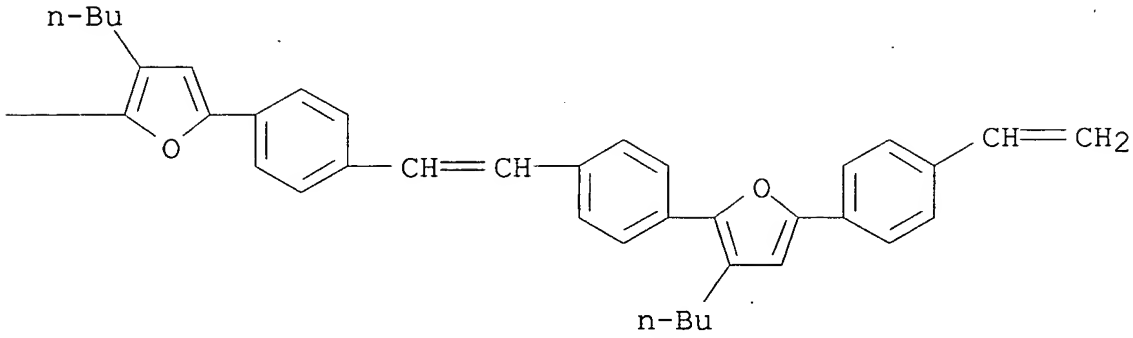
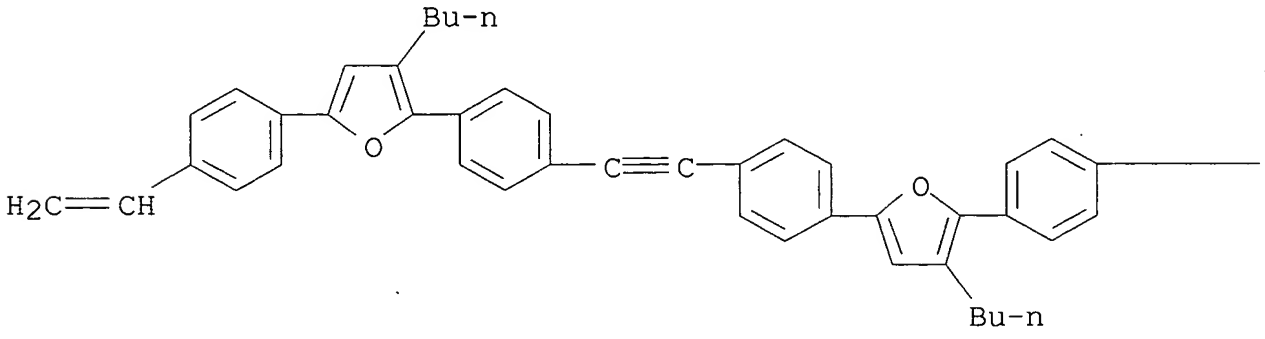


RN 515139-48-7 HCA
CN Furan, 2,2'-(1,4-phenylene)bis[3-butyl-5-[4-[[4-[3-butyl-5-(4-ethenylphenyl)-2-furanyl]phenyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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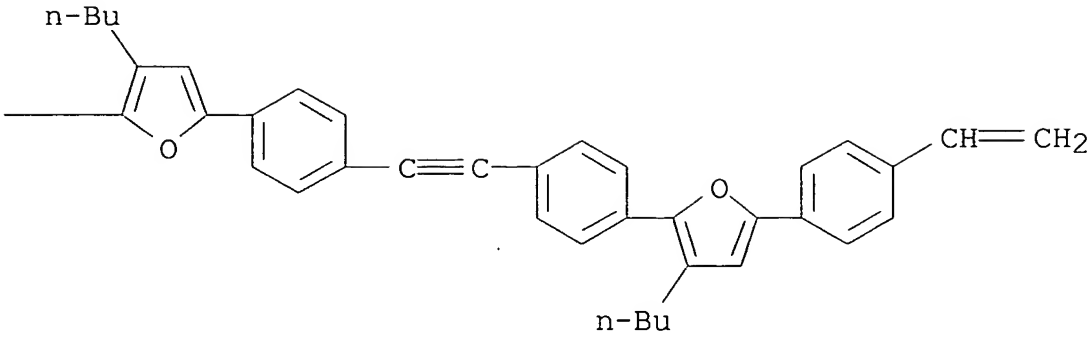
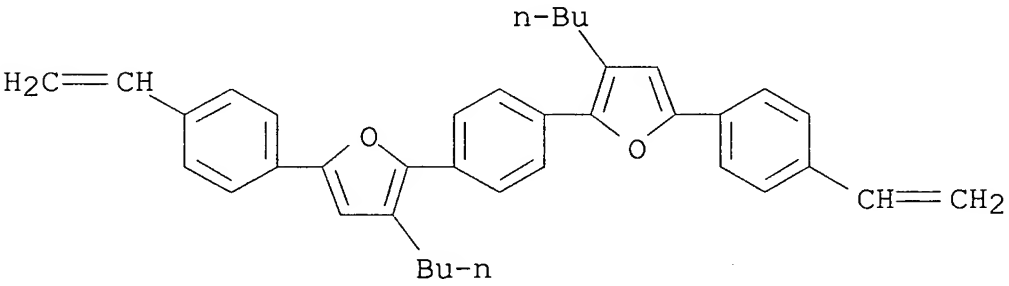
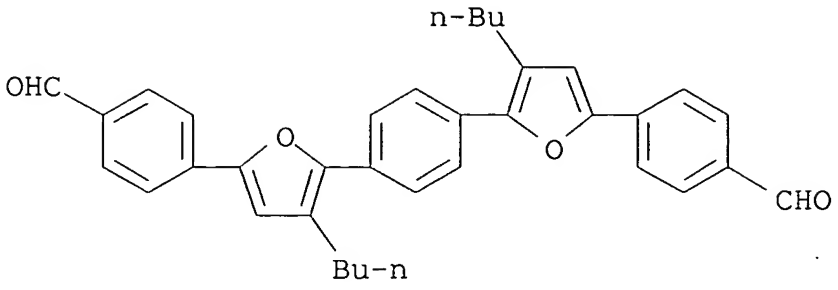


IT **282096-58-6P 515139-36-3P 515139-38-5P 515139-40-9P 515139-41-0P 515139-42-1P 551897-93-9P**
(preparation of alternating benzene-furan oligomers via reaction of propargylic dithioacetal with butyllithium followed by reaction with aldehydes and photophys. and electrochem. of products useful for mol. wire applications)

RN 282096-58-6 HCA
CN Furan, 2,2'-(1,4-phenylene)bis[3-butyl-5-(4-ethenylphenyl)- (9CI) (CA INDEX NAME)

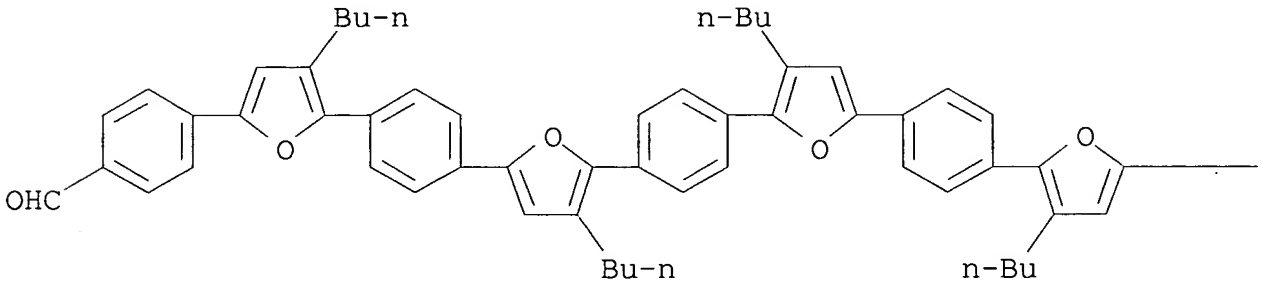


RN 515139-36-3 HCA
CN Benzaldehyde, 4,4'-[1,4-phenylenebis(4-butyl-5,2-furandiyl)]bis- (9CI) (CA INDEX NAME)

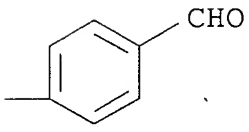


RN 515139-38-5 HCA
CN Benzaldehyde, 4,4'-[1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylene(4-butyl-5,2-furandiyl)]]bis- (9CI) (CA INDEX NAME)

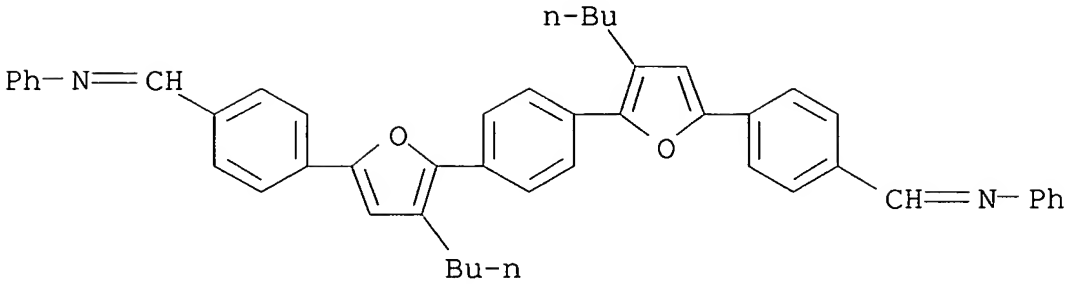
PAGE 1-A



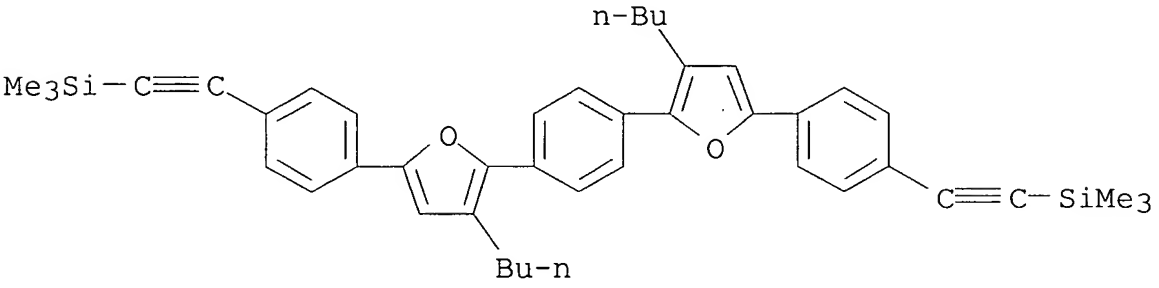
PAGE 1-B



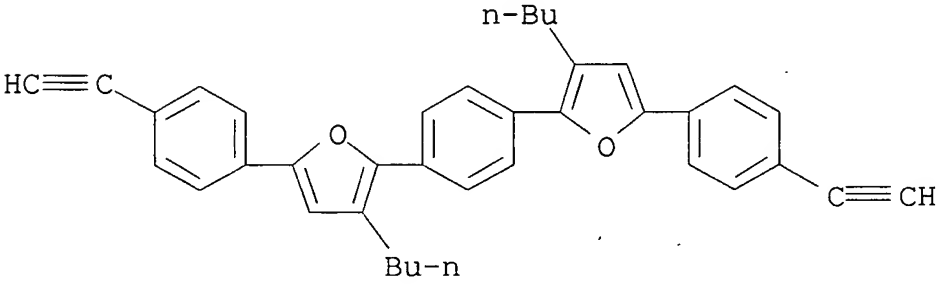
RN 515139-40-9 HCA
CN Benzenamine, N,N'-[1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylenemethylidyne]]bis- (9CI) (CA INDEX NAME)



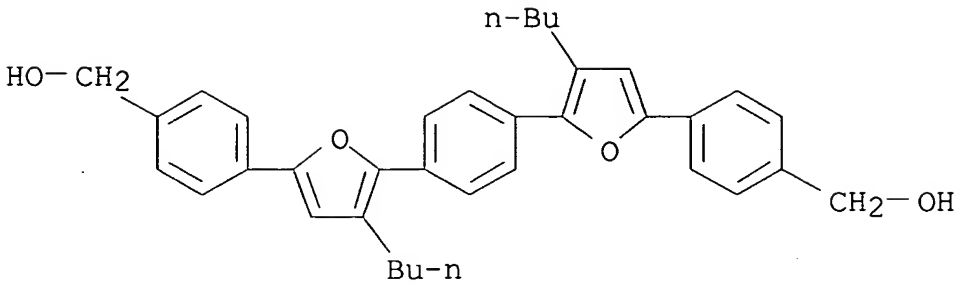
RN 515139-41-0 HCA
CN Silane, [1,4-phenylenebis[(4-butyl-5,2-furandiyl)-4,1-phenylene-2,1-ethynediyl]]bis[trimethyl- (9CI) (CA INDEX NAME)



RN 515139-42-1 HCA
CN Furan, 2,2'-(1,4-phenylene)bis[3-butyl-5-(4-ethynylphenyl)- (9CI) (CA INDEX NAME)



RN 551897-93-9 HCA
CN Benzenemethanol, 4,4'-[1,4-phenylenebis(4-butyl-5,2-furandiyl)]bis- (9CI) (CA INDEX NAME)



CC 27-6 (Heterocyclic Compounds (One Hetero Atom))

IT **515139-35-2P 515139-37-4P 515139-44-3P**
515139-45-4P
(preparation of alternating benzene-furan oligomers via reaction of propargylic dithioacetal with butyllithium followed by reaction with aldehydes and photophys. and electrochem. of products useful for mol. wire applications)

IT **515139-39-6P 515139-43-2P 515139-46-5P**
515139-47-6P 515139-48-7P
(preparation of alternating benzene-furan oligomers via reaction of propargylic dithioacetal with butyllithium followed by reaction with aldehydes and photophys. and electrochem. of products useful for mol. wire applications)

IT **282096-58-6P** 515139-34-1P **515139-36-3P**
515139-38-5P 515139-40-9P 515139-41-0P
515139-42-1P 551897-93-9P
(preparation of alternating benzene-furan oligomers via reaction of propargylic dithioacetal with butyllithium followed by reaction with aldehydes and photophys. and electrochem. of products useful for mol. wire applications)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 5 OF 35 HCA COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 138:89634 HCA

TITLE: Combining Furan Annulation, Heck Reaction, and Sonogashira Coupling for the Synthesis of Oligoaryls

AUTHOR(S): Liu, Ching-Yuan; Luh, Tien-Yau

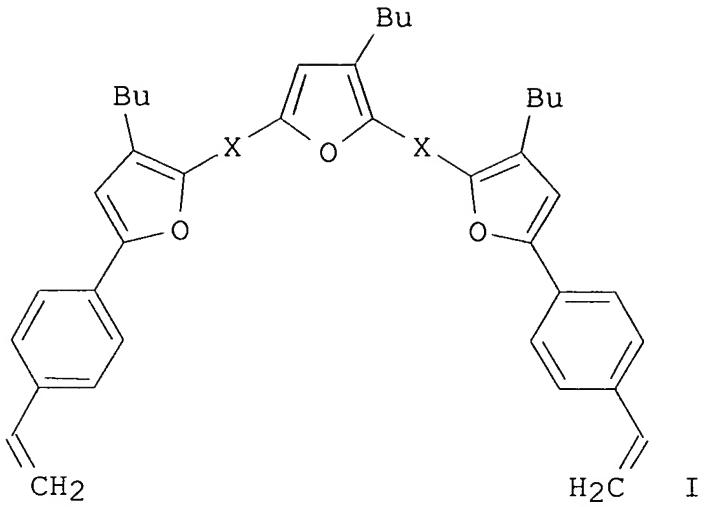
CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan

SOURCE: Organic Letters (2002), 4(24), 4305-4307
CODEN: ORLEF7; ISSN: 1523-7060

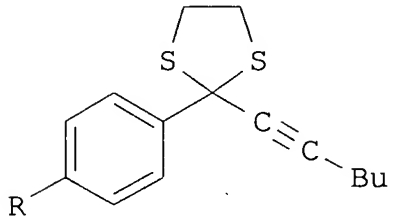
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:89634
GI



I



II

AB Oligoaryl derivs. such as I (X = 4-C6H4C.tplbond.C-4-C6H4) consisting of furan, p-phenylene, ethynediyl, and ethenediyl groups are prepared from alkynyl dithiolanes II (R = Me3SiC.tplbond.C, H2C:CH) by a furan annulation reaction with aromatic aldehydes followed either by Heck or Sonogashira coupling reactions with aromatic aldehydes to provide di(formylphenyl)furans which can undergo further reaction with II to provide oligoaryls of defined length. Alkynyldithiolanes II undergo fragmentation with butyllithium to provide allenyllithium reagents which add to aryl aldehydes; the intermediate aldehyde addition products cyclize upon treatment with trifluoroacetic acid to give diarylfurans. When an alkynylbenzaldehyde is used as addition partner, deprotection of the

alkyne followed by treatment with p-bromobenzaldehyde in the presence of bid(triphenylphosphine)palladium dichloride, copper (I) iodide, and triethylamine in acetonitrile provides an aldehyde which can undergo a second addition-cyclocondensation reaction. Heck reaction of p-bromobenzaldehyde with a vinylated oligoaryl in the presence of palladium acetate and triphenylphosphine in acetonitrile provides unsatd. vinyl-containing oligoaryls. Oligoaryls such as I are tested for their absorption and emission wavelengths as well as their fluorescence quantum yields; the extended vinylene-containing polymer decomposed under exposure to ambient light.

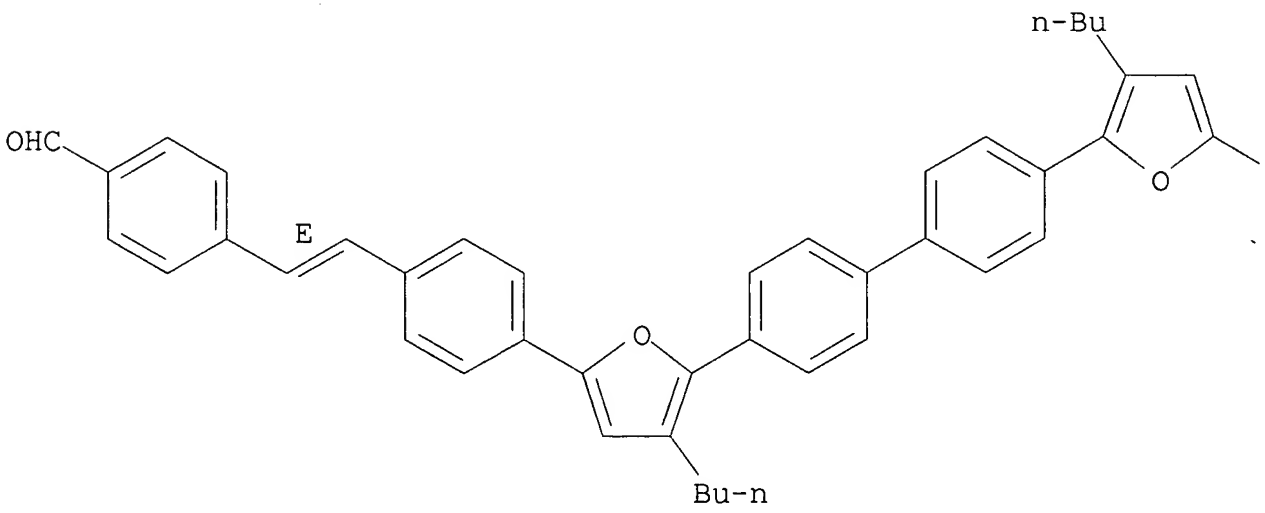
IT **484067-74-5P**
(preparation and photophys. properties of furan-containing oligoaryls by cyclocondensation of allenyllithium reagents generated from alkynyldithiolanes and aryl aldehydes followed by either Heck or Sonogashira coupling reactions)

RN 484067-74-5 HCA

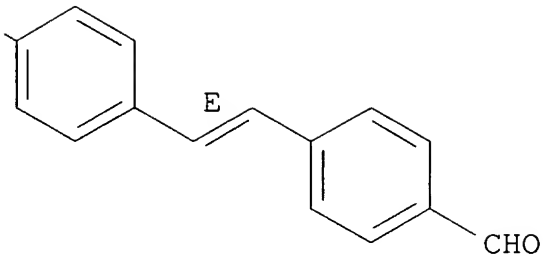
CN Benzaldehyde, 4,4'-[[1,1'-biphenyl]-4,4'-diylbis[(4-butyl-5,2-furandiyl)-4,1-phenylene-(1E)-2,1-ethenediyl]]bis- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



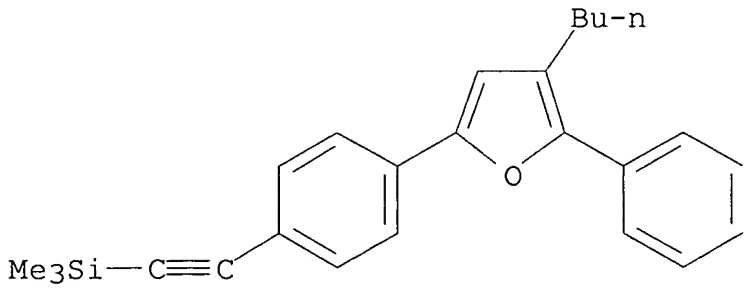
PAGE 1-B



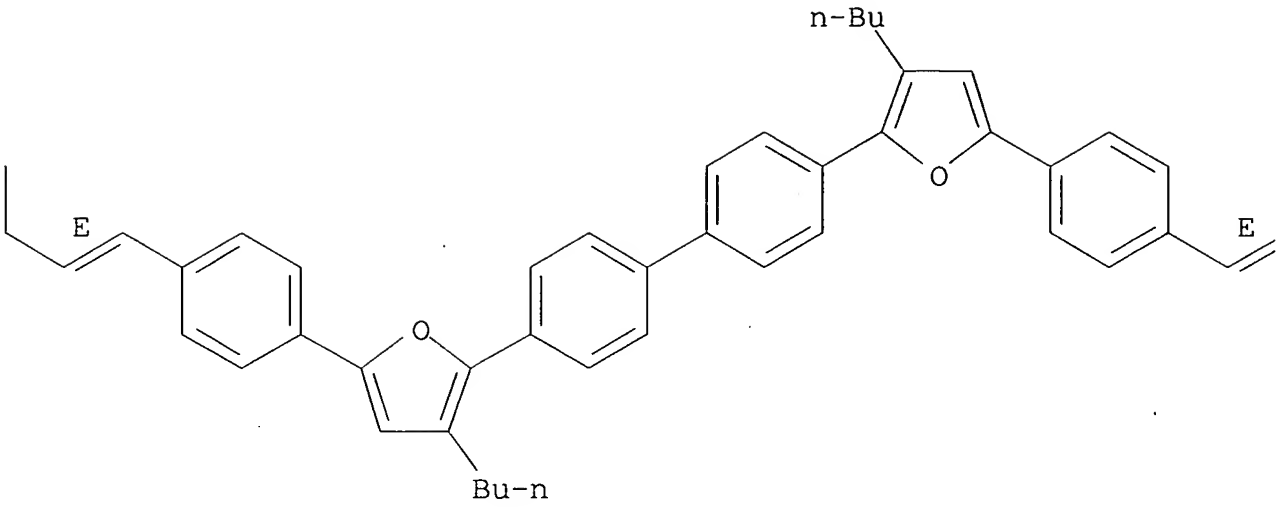
IT **484067-77-8P**
(preparation and photophys. properties of furan-containing oligoaryls by
cyclocondensation of allenyllithium reagents generated from alkynyldithiolanes and aryl aldehydes followed by either Heck or Sonogashira coupling reactions)
RN 484067-77-8 HCA
CN Silane, [[1,1'-biphenyl]-4,4'-diylbis[(4-butyl-5,2-furandiyl)-4,1-phenylene-(1E)-2,1-ethenediyl-4,1-phenylene(4-butyl-5,2-furandiyl)-4,1-phenylene-2,1-ethynediyl]]bis[trimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

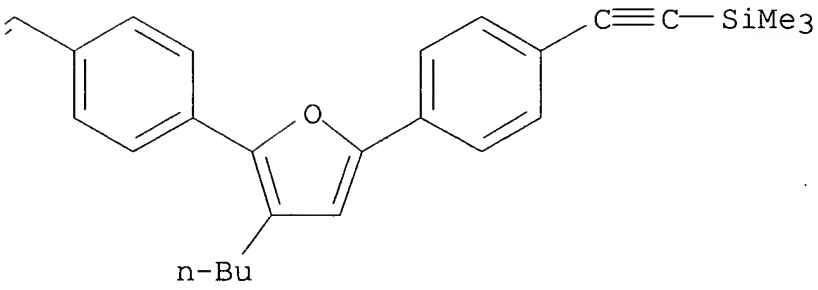
PAGE 1-A



PAGE 1-B



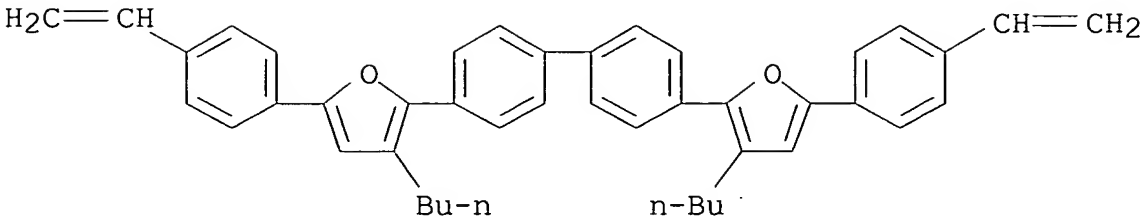
PAGE 1-C



IT **282096-60-0P**
(preparation of furan-containing oligoaryls by cyclocondensation of allenyllithium reagents generated from alkynyldithiolanes and aryl aldehydes followed by either Heck or Sonogashira coupling reactions)

RN 282096-60-0 HCA

CN Furan, 2,2'-[1,1'-biphenyl]-4,4'-diylbis[3-butyl-5-(4-ethenylphenyl)- (9CI) (CA INDEX NAME)



CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
IT **484067-74-5P** 484067-75-6P
(preparation and photophys. properties of furan-containing oligoaryls by
cyclocondensation of allenyllithium reagents generated from alkynyldithiolanes and aryl aldehydes followed by either Heck or Sonogashira coupling reactions)
IT 484067-76-7P **484067-77-8P**
(preparation and photophys. properties of furan-containing oligoaryls by
cyclocondensation of allenyllithium reagents generated from alkynyldithiolanes and aryl aldehydes followed by either Heck or Sonogashira coupling reactions)
IT **282096-60-0P** 484067-72-3P 484067-73-4P
(preparation of furan-containing oligoaryls by cyclocondensation of allenyllithium reagents generated from alkynyldithiolanes and aryl aldehydes followed by either Heck or Sonogashira coupling reactions)
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 6 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 138:74688 HCA
TITLE: Novel fluorescent quater- and quinquifurans: syntheses and photophysical properties
AUTHOR(S): Kauffman, Joel M.; Moyna, Guillermo
CORPORATE SOURCE: Univ. of the Scientific in Philadelphia, Philadelphia, PA, 19104-4495, USA
SOURCE: Journal of Heterocyclic Chemistry (2002), 39(5), 981-988
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:74688
AB In the quest for fast fluors for use in wave-shifting polystyrene fibers, sym. oligofurans were investigated. Furan moieties were

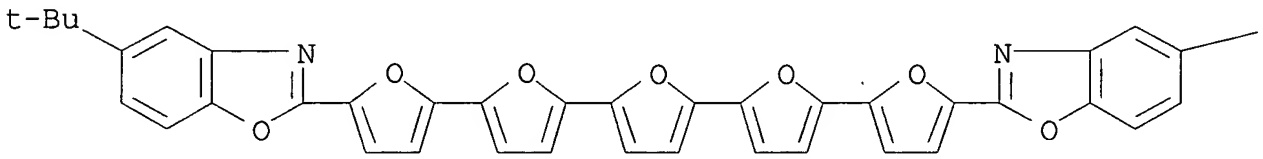
coupled by means of the Ullmann reaction or by palladium-catalyzed unsym. coupling; the latter gave higher yields. While the benzoxazole-terminated quater- and quinquifurans we prepared were both stable and fast, exhibiting a green fluorescence and decay times of about 2.4 ns, they were inferior to other types of fluors in solubility
and emission intensity when incorporated into polystyrene..

IT **256339-27-2P 479668-75-2P**
(dye; preparation and fluorescence of benzimidazole-terminated oligofurans)

RN 256339-27-2 HCA

CN Benzoxazole, 2,2'-[2,2':5',2'':5'',2''':5''',2''''-quinquefuran]-5,5''''-diylbis[5-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

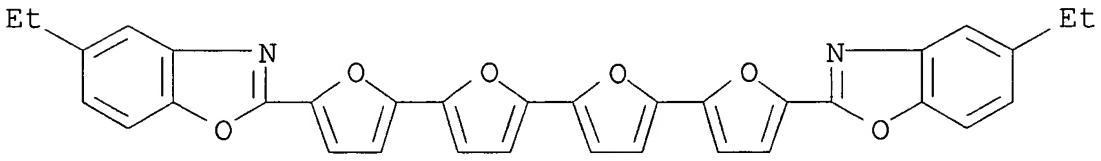


PAGE 1-B

Bu-t

RN 479668-75-2 HCA

CN Benzoxazole, 2,2'-[2,2':5',2'':5'',2'''-quaterfuran]-5,5'''-diylbis[5-ethyl- (9CI) (CA INDEX NAME)



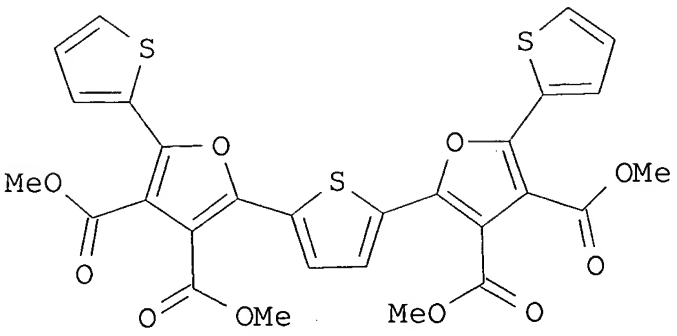
CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 28, 73

IT **256339-27-2P 479668-75-2P**
(dye; preparation and fluorescence of benzimidazole-terminated oligofurans)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE

IN THE RE FORMAT

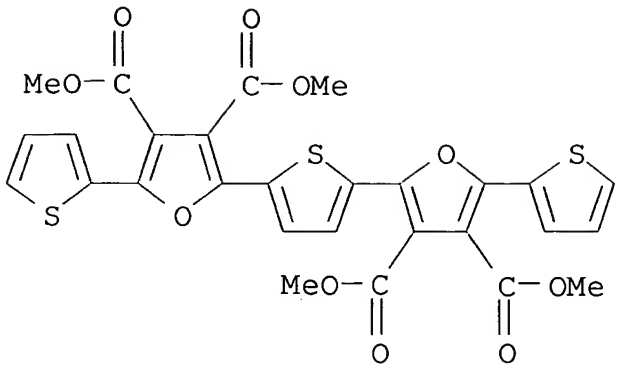
L36 ANSWER 7 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 138:55820 HCA
TITLE: Controlled synthesis of functionalized mixed thiophene/furan oligomers
AUTHOR(S): Garzino, Frederic; Meou, Alain; Brun, Pierre
CORPORATE SOURCE: Lab. de Synthese Organique Selective, GCOMM, UMR-CNRS 6114, Univ. de la Mediterranee, Marseille, F-13288, Fr.
SOURCE: Helvetica Chimica Acta (2002), 85(7), 1989-1998
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:55820
GI



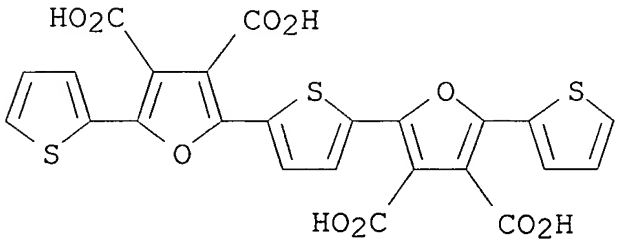
I

AB A novel and simple synthetic route for the preparation of a series of functionalized mixed thiophene/furan oligomers, e.g I, is described. This method, involving a Mn(OAc)3-mediated oxidative addition of β-thienyl-β-keto esters to Me 3-thienylprop-2-enoates, allows the construction of highly functionalized heteropolyarom. oligomers possessing various chain lengths. Moreover, the straightforward transformation of the carbonyl functions appended to the furan rings leads to polycarboxylic acid precursors of H2O-soluble conducting polymers.

IT **479421-47-1P**
(controlled synthesis of functionalized mixed thiophene/furan oligomers)
RN 479421-47-1 HCA
CN 3,4-Furandicarboxylic acid, 2,2'-(2,5-thiophenediyl)bis[5-(2-thienyl)-, tetramethyl ester (9CI) (CA INDEX NAME)



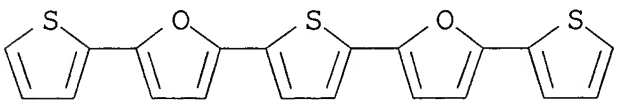
IT **479421-59-5P**
(controlled synthesis of functionalized mixed thiophene/furan oligomers)
RN 479421-59-5 HCA
CN 3,4-Furandicarboxylic acid, 2,2'-(2,5-thiophenediyl)bis[5-(2-thienyl)- (9CI) (CA INDEX NAME)



CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
IT 57502-38-2P 76010-70-3P 134568-16-4P 185515-21-3P
479421-44-8P 479421-45-9P 479421-46-0P **479421-47-1P**
479421-48-2P 479421-49-3P 479421-50-6P 479421-51-7P
479421-52-8P 479421-55-1P 479421-56-2P
(controlled synthesis of functionalized mixed thiophene/furan oligomers)
IT 479421-53-9P 479421-54-0P 479421-57-3P 479421-58-4P
479421-59-5P
(controlled synthesis of functionalized mixed thiophene/furan oligomers)
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 8 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 138:55608 HCA
TITLE: Photophysical studies of mixed furan, pyrrole, and thiophene-containing oligomers with three

and five rings
AUTHOR(S): Seixas de Melo, J.; Elisei, Fausto; Becker, Ralph S.
CORPORATE SOURCE: Chemistry Department, University of Coimbra, Coimbra, 3004-535, Port.
SOURCE: Journal of Chemical Physics (2002), 117(9), 4428-4435
CODEN: JCPSA6; ISSN: 0021-9606
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The photophysics of several oligomers containing mixed furan, pyrrole, and thiophene heterocyclic systems is reported. The mixed systems contain three rings and five rings of the heterocycles. Comprehensive spectroscopic and photophys. data were obtained and all of the rate consts. kF, kIC, and kISC were evaluated. The lowest singlet excited state is of (1)B-like origin in any solvent. It is possible to have a reasonable understanding of the photophysics of the mixed ring systems compared to all the thiophene analogs if it is considered that some π-electron decoupling occurs at the site of the pyrrole or furan substitution, although this cannot be the total answer, as is discussed.
IT **157667-21-5**
(UV absorption and emission spectra of mixed furan, pyrrole, and thiophene-containing oligomers with three and five rings)
RN 157667-21-5 HCA
CN Furan, 2,2'-(2,5-thiophenediyl)bis[5-(2-thienyl)- (9CI) (CA INDEX NAME)



CC 22-9 (Physical Organic Chemistry)
Section cross-reference(s): 73
IT 1081-34-1, 2,2':5',2''-Terthiophene 88089-34-3 89814-62-0
155042-09-4 157667-20-4 **157667-21-5** 161869-63-2
161869-64-3 161869-65-4
(UV absorption and emission spectra of mixed furan, pyrrole, and thiophene-containing oligomers with three and five rings)
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 9 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 137:200939 HCA
TITLE: Influence of building block aromaticity in the

determination of electronic properties of five-membered heterocyclic oligomers

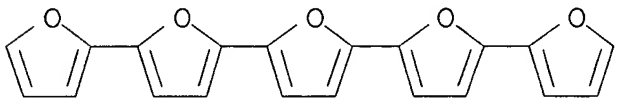
AUTHOR(S): Delaere, David; Nguyen, Minh Tho; Vanquickenborne, Luc G.
CORPORATE SOURCE: Department of Chemistry, University of Leuven, Louvain, B-3001, Belg.

SOURCE: Physical Chemistry Chemical Physics (2002), 4(9), 1522-1530
CODEN: PPCPFQ; ISSN: 1463-9076
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

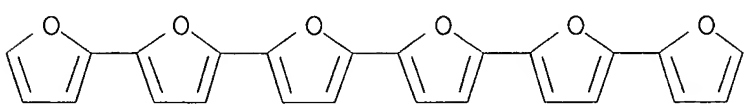
AB This theor. study investigates the influence of the building block aromaticity in the determination of electronic properties of five-membered heterocyclic oligomers. More specifically, we considered some fundamental energetic and electronic properties such as energy gaps, vertical ionization energies and static polarizability tensors of oligomers (up to octamers) built from five-membered heterocycles such as cyclopentadiene, pyrrole, furan, silole, (planar) phosphole and thiophene. Our computations are based on ab initio quantum mech. methods including (time-dependent) d. functional theory. We have chosen NICS as a quant. criterion for measuring aromaticity and making a distinction between aromatic and non-aromatic building blocks.

IT **137040-24-5 174895-49-9 453507-77-2**
453507-78-3
(influence of building block aromaticity in the determination of electronic properties of five-membered heterocyclic oligomers)

RN 137040-24-5 HCA
CN 2,2':5',2'':5'',2''':5''',2''''-Quinquefuran (9CI) (CA INDEX NAME)

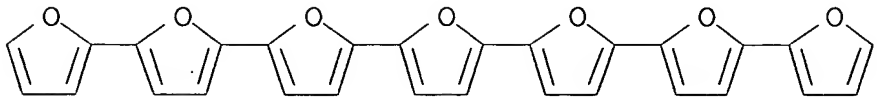


RN 174895-49-9 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2'''''-Sexifuran (9CI) (CA INDEX NAME)

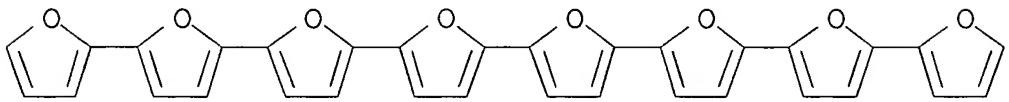


RN 453507-77-2 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2''''':5''''',2'''''':

Septifuran (9CI) (CA INDEX NAME)



RN 453507-78-3 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2''''':5''''',2'''''':5'''''',
2''''''':5'''''''-Octifuran (9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)
Section cross-reference(s): 35
IT 109-97-7, Pyrrole 110-00-9, Furan 110-02-1, Thiophene
492-97-7, 2,2'-Bithiophene 542-92-7, Cyclopentadiene, properties
1081-34-1, 2,2':5',2''-Terthiophene 3260-45-5,
2,2':5',2''-Ter-1H-pyrrole 4723-64-2, Silole 5632-29-1,
2,2':5',2'':5'',2'''-Quaterthiophene 5660-45-7 5905-00-0,
2,2'-Bifuran 10087-64-6, 2,2'-Bi-1H-pyrrole 21423-87-0,
Bi-1,3-cyclopentadien-1-yl 62889-09-2, 2,2':5',2''-Terfuran
80421-31-4, 2,2':5',2'':5'',2'''-Quaterfuran 86100-63-2
86450-98-8, 2,2':5',2'':5'',2'''-Quater-1H-pyrrole 88493-55-4
108664-04-6 108664-05-7 113728-71-5 **137040-24-5**
152040-64-7 152040-65-8 173413-62-2, Bisilacyclopenta-2,4-dien-2-
yl **174895-49-9** 205824-76-6 218965-94-7,
1,1':4',1''-Ter-1,3-cyclopentadiene 218965-95-8 218965-96-9
218965-97-0, 2,2':5',2''-Tersilacyclopenta-2,4-diene 218965-98-1
218965-99-2 218966-00-8 453507-71-6 453507-72-7 453507-73-8
453507-74-9 **453507-77-2** **453507-78-3**
(influence of building block aromaticity in the determination of electronic properties of five-membered heterocyclic oligomers)
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 10 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 136:38057 HCA
TITLE: Metallocene compound, olefin polymerization catalyst containing the compound, and method for producing an olefin polymer by use of the catalyst
INVENTOR(S): Nakano, Masato; Ushioda, Tsutomu; Yamazaki, Hiroshi; Uwai, Toshihiro; Kimura, Masami; Ohgi,

Yoshiyuki; Yamamoto, Kiyomi
PATENT ASSIGNEE(S): Chisso Corporation, Japan
SOURCE: U.S. Pat. Appl. Publ., 26 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2001053833	A1	20011220	US 2001-861726	20010522
JP 2002047313	A2	20020212	JP 2000-321373	20001020
JP 2002128832	A2	20020509	JP 2000-321376	20001020
JP 2002194016	A2	20020710	JP 2001-149062	20010518
DE 10125356	A1	20020124	DE 2001-10125356	20010523

PRIORITY APPLN. INFO.:

JP 2000-151673	A	20000523
JP 2000-151674	A	20000523
JP 2000-321373	A	20001020
JP 2000-321374	A	20001020
JP 2000-321376	A	20001020

AB A metallocene compound useful as catalyst for manufacturing of polyolefins

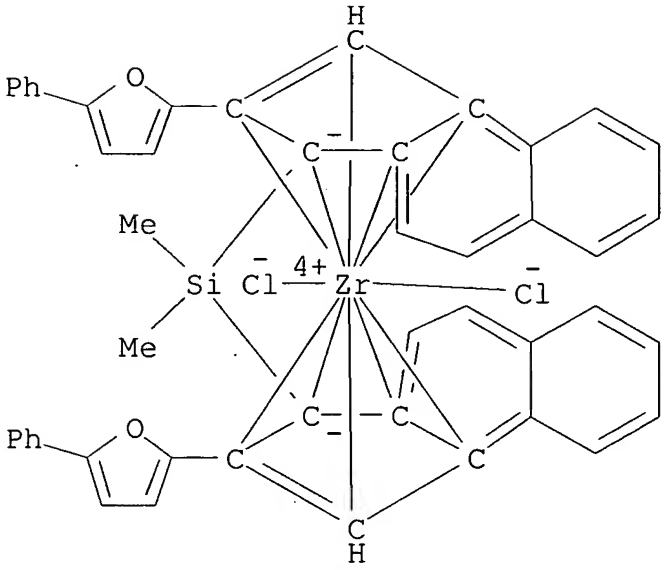
with high mol. weight and high stereoregularity has the following formula: Q(C5H4-m R1m)(C5H4-nR2n)MXY wherein (C5H4-m R1m) and (C5H4-n R2n) each independently represent a cyclopentadienyl group; C5H4-m and C5H4-n each independently represent a cyclopentadienyl ring; m represents an integer of 1-3; n represents an integer of 2 or 3; R1 and R2 are each independently a substituent bonded resp. to C5H4-m and C5H4-n , and represent a hydrocarbon group of 1-20 carbon atoms, a silicon-containing hydrocarbon group of 1-20 carbon atoms or a heteroarom. group; each R1m and each R2n may be the same or different; one pair of R2's in the R2n are bonded to each other to form at least one ring; Q represents a divalent group for crosslinking (C5H4-m R1m) and (C5H4-n R2n); M represents a titanium atom, a zirconium atom or a hafnium atom; and X and Y are the same or different and each a hydrogen atom, a halogen atom or a hydrocarbon group. Thus, propylene was introduced under 0.3 MPa to a mixture of 1L toluene solution containing methylaluminoxane-rac and 3 mL rac-dimethylsilylene bis(2-(2-(5-methyl)furyl)indenyl)zirconium dichloride-toluene solution and polymerized for 1 h to give 8.7 g propylene homopolymer having melt flow rate 0.004 g/10 min, isotactic pentad ratio 0.928, isotactic triad ratio 0.946, weight-average mol. weight 1.61 + 106 g/mol, Mw/Mn 3.0, and m.p. 146.2°.

IT **380911-00-2 380911-07-9 380911-14-8**
(metallocene catalysts for polymerization of olefins to high-mol.-weight polymers with high stereoregularity)

RN 380911-00-2 HCA
CN Zirconium, dichloro[rel-(1R,1'R)-(dimethylsilylene)bis[(1,2,3,3a,7a-η)-4-phenyl-2-(5-phenyl-2-furanyl)-1H-inden-1-ylidene]]- (9CI) (CA INDEX NAME)

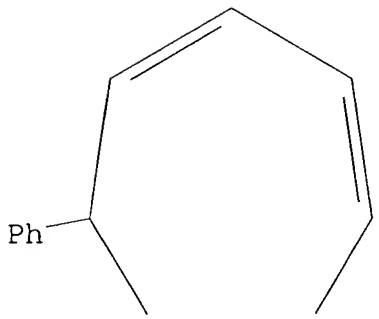
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 380911-07-9 HCA
CN Zirconium, dichloro[rel-(3R,3'R)-(dimethylsilylene)bis[(1,2,3,3a,9b-η)-2-(5-phenyl-2-furanyl)-3H-benz[e]inden-3-ylidene]]- (9CI) (CA INDEX NAME)

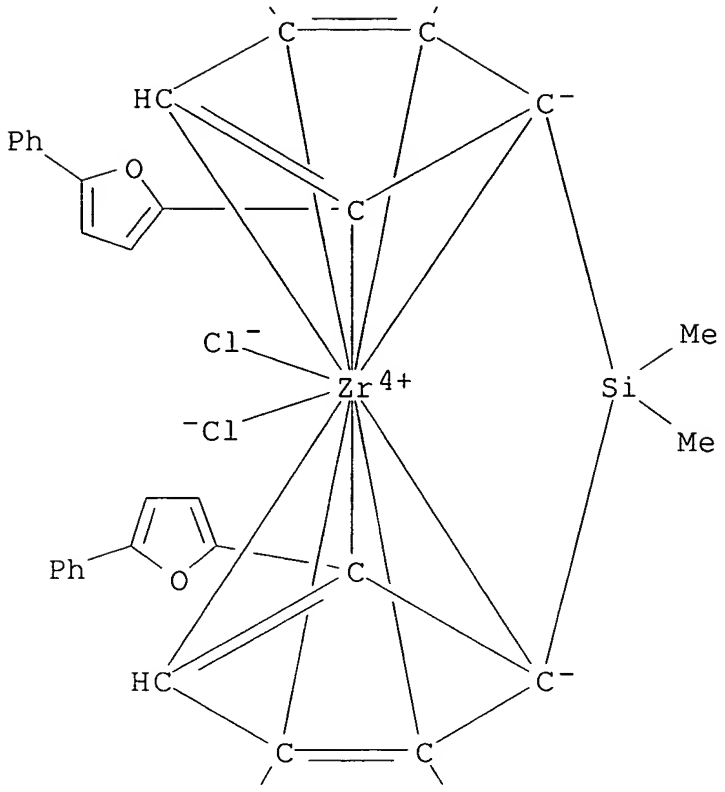


RN 380911-14-8 HCA
CN Zirconium, dichloro[(dimethylsilylene)bis[(1,2,3,3a,8a-η)-4-phenyl-2-(5-phenyl-2-furanyl)-1(4H)-azulenylidene]]- (9CI) (CA INDEX NAME)

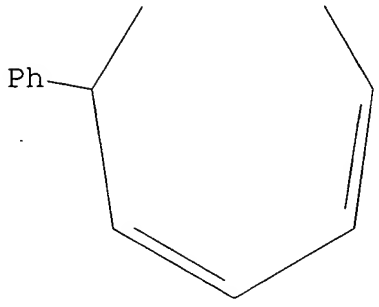
PAGE 1-A



PAGE 2-A



PAGE 3-A



IT **380910-91-8P**
(metallocene catalysts for polymerization of olefins to high-mol.-weight
polymers with high stereoregularity)
RN 380910-91-8 HCA

CN Zirconium, dichloro[rel-(1R,1'R)-(dimethylsilylene)bis[(1,2,3,3a,7a-η)-2-(5-phenyl-2-furanyl)-1H-inden-1-ylidene]]- (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IC ICM C08F004-44
NCL 526127000
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29
IT 380910-92-9 380910-93-0 380910-94-1 380910-95-2 380910-96-3
380910-97-4 380910-98-5 380910-99-6 **380911-00-2**
380911-01-3 380911-02-4 380911-03-5 380911-04-6 380911-05-7
380911-06-8 **380911-07-9** 380911-08-0 380911-09-1
380911-10-4 380911-11-5 380911-12-6 380911-13-7
380911-14-8 380911-15-9 380911-16-0 380911-17-1
380911-18-2
(metallocene catalysts for polymerization of olefins to high-mol.-weight
polymers with high stereoregularity)
IT 380910-82-7P 380910-85-0P 380910-88-3P **380910-91-8P**
(metallocene catalysts for polymerization of olefins to high-mol.-weight
polymers with high stereoregularity)

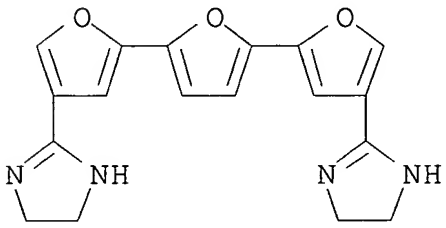
L36 ANSWER 11 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 136:170 HCA
TITLE: Novel dications with unfused aromatic systems: trithiophene and trifuran derivatives of furimidazoline
AUTHOR(S): Bilik, Petr; Tanious, Farial; Kumar, Arvind; Wilson, W. David; Boykin, David W.; Colson, Pierre; Houssier, Claude; Facompre, Michael; Tardy, Christelle; Bailly, Christian
CORPORATE SOURCE: Department of Chemistry, Georgia State University, Atlanta, GA, 30303, USA
SOURCE: ChemBioChem (2001), 2(7-8), 559-569
CODEN: CBCHFX; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We report the synthesis, interaction with DNA, topoisomerase II inhibition, and cytotoxicity of two novel unfused aromatic dications derived from the antimicrobial agent furimidazoline. The central diphenylfuran core of furimidazoline has been replaced with a trithiophene (DB358) or a trifuran (DB669) unit and the terminal imidazoline groups were preserved. The strength and mode of binding of the drugs to nucleic acids were investigated by complementary spectroscopic techniques including spectrophotometric, surface plasmon resonance, circular and linear dichroism measurements. The

trifuran derivative forms intercalation complexes with double-stranded DNA, whereas the mode of binding of the trithiophene derivative varies depending on the drug/DNA ratio, as independently confirmed by NMR spectroscopic studies performed with (A-T)7 and (G-C)7 oligomers. Two-dimensional NMR data provided a mol. model for the binding of DB358 within the minor groove of the AATT sequence of the decanucleotide d(GCGAATTCGC)2. DNase I footprinting expts. confirmed the sequence-dependent binding of DB358 to DNA. The trithiophene derivative interacts preferentially with AT-rich sequences at low concns., but can accommodate GC sites at higher concns. DNA relaxation assays revealed that DB358 stimulated DNA cleavage by topoisomerase II, in contrast to DB669. The substitution of N-alkylamidines for the imidazoline terminal groups abolished the capacity of the drug to poison topoisomerase II. At the cellular level, flow cytometry anal. indicated that DB358, which is about six times more cytotoxic than the trifuran analog, induced a significant accumulation of HL-60 human leukemia cells in the G2/M phase. The incorporation of thiophene heterocycles appears as a convenient procedure to limit the strict AT selectivity of dications containing an extended unfused aromatic system and to design cytotoxic DNA intercalating agents acting as poisons for human topoisomerase II.

IT **375390-94-6P**, DB 669
(trithiophene and trifuran derivs. of furimidazoline synthesis, interaction with DNA, topoisomerase II inhibition and cytotoxicity)

RN 375390-94-6 HCA

CN 1H-Imidazole, 2,2'-[2,2':5',2''-terfuran]-4,4''-diylbis[4,5-dihydro- (9CI) (CA INDEX NAME)

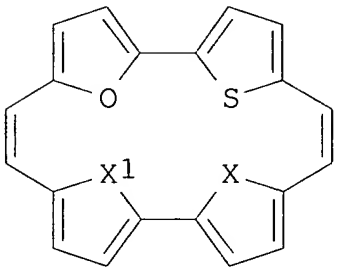


CC 1-3 (Pharmacology)

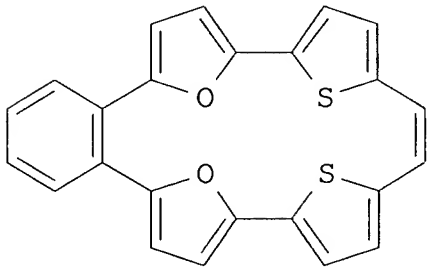
IT 375390-93-5P, DB 358 **375390-94-6P**, DB 669
(trithiophene and trifuran derivs. of furimidazoline synthesis, interaction with DNA, topoisomerase II inhibition and cytotoxicity)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 12 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 134:193268 HCA
TITLE: First synthesis of dioxadithiaporphycene with a benzene ring fused onto the double bond
AUTHOR(S): Dai, W.-M.; Mak, W. L.
CORPORATE SOURCE: Department of Chemistry, The Hong Kong University of Science and Technology, Kowloon, Hong Kong SAR, Hong Kong
SOURCE: Tetrahedron Letters (2000), 41(52), 10277-10280
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:193268
GI



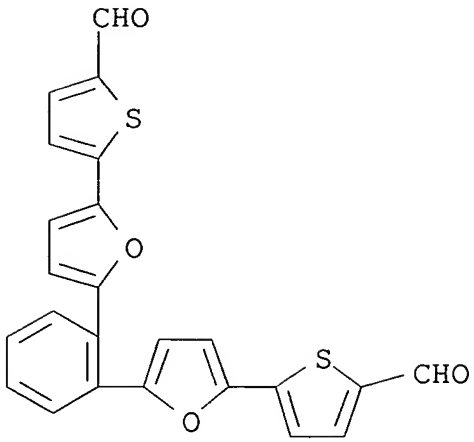
I



II

AB Dioxadithiaporphycenes I (X = O, X1 = S; X = S, X1 = O) were synthesized by using the Suzuki cross-coupling and McMurry coupling reactions as the key steps. This approach provided an access to the first dioxadithiaporphycene derivative II with a benzene ring fused onto the double bond.

IT **326925-42-2P**
(synthesis of dioxadithiaporphycenes and a benzodioxadithiaporphycene via Suzuki cross-coupling and McMurry coupling reactions)
RN 326925-42-2 HCA
CN 2-Thiophenecarboxaldehyde, 5,5'-(1,2-phenylenedi-5,2-furandiyl)bis- (9CI) (CA INDEX NAME)



CC 26-7 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 28
IT 27521-80-8P 326925-40-0P 326925-41-1P **326925-42-2P**
(synthesis of dioxadithiaporphycenes and a benzodioxadithiaporphycene via Suzuki cross-coupling and McMurry coupling reactions)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

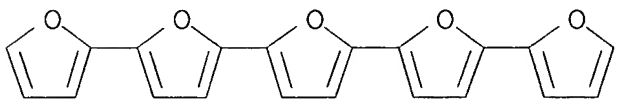
L36 ANSWER 13 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 133:237513 HCA
TITLE: Comprehensive Investigation of the Photophysical Behavior of Oligopolyfurans
AUTHOR(S): Seixas de Melo, J.; Elisei, Fausto; Gartner, Carlos; Aloisi, Gian Gaetano; Becker, Ralph S.
CORPORATE SOURCE: Chemistry Department, University of Coimbra, Coimbra, 3049, Port.
SOURCE: Journal of Physical Chemistry A (2000), 104(30), 6907-6911
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The photophys. properties of (oligo)polyfurans (Fn, where n = 1-5 represents the number of rings) are presented for the 1st time for 2-4 rings and compared to parallel data for the corresponding (oligo)polythiophenes (Tn). The quantum yields of fluorescence of the polyfurans are consistently considerably greater (5-50-fold), and that of the triplet occupation, considerably smaller (2.5-4) than for the polythiophenes. The kF of the Fn set vary from about equal (n = 4) to ≈4-fold greater (n = 2) than for the Tn

set. The kISC of the Fn set are from 10-25-fold smaller than for the Tn set. The Fn set shows very little internal conversion (except some for F2) and less than for the Tn set. Triplet lifetimes of the Fn set are ≈3 fold less than for the Tn set. The lowest excited singlet state of the polyfurans is of 1Bu (or 1B1) character and not 1Ag. The magnitude of the intersystem crossing is essentially constant as a function of n for the Fn set whereas there is a large decrease for the Tn set as n increases. This indicates a difference in the mechanism for intersystem crossing as is discussed. The π-delocalization is greater for the Tn set than for the Fn set. It is not possible to clearly distinguish whether cis and trans conformers simultaneously exist (most likely for F2), or the magnitude of inter-ring bond twisting but the latter appears to be ≤20-30 degrees and the virtual mols. at 77 K are clearly more planar than at room temperature

IT **137040-24-5**
(comprehensive study of photophys. behavior of oligopolyfurans)

RN 137040-24-5 HCA

CN 2,2':5',2'':5'',2''':5''',2''''-Quinquefuran (9CI) (CA INDEX NAME)



CC 22-9 (Physical Organic Chemistry)
Section cross-reference(s): 36, 73, 74

IT 110-00-9, Furan 110-02-1, Thiophene 492-97-7, 2,2'-Bithiophene 1081-34-1, 2,2':5',2''-Terthiophene 5632-29-1, 2,2':5',2'':5'',2'''-Quaterthiophene 5660-45-7 5905-00-0, 2,2'-Bifuran 62889-09-2, 2,2':5',2''-Terfuran 80421-31-4, 2,2':5',2'':5'',2'''-Quaterfuran **137040-24-5**
(comprehensive study of photophys. behavior of oligopolyfurans)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 14 OF 35 HCA COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 132:129270 HCA

TITLE: Computational methods as an aid in the design of fluorophores with predictable absorption and emission wavelengths

AUTHOR(S): Fabian, Walter M. F.; Kauffman, Joel M.

CORPORATE SOURCE: Institut fur Organische Chemie, Karl-Franzens Universitat Graz, Graz, A-8010, Austria

SOURCE: Journal of Luminescence (1999), 85(1-3), 137-148
CODEN: JLUMA8; ISSN: 0022-2313

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal
LANGUAGE: English

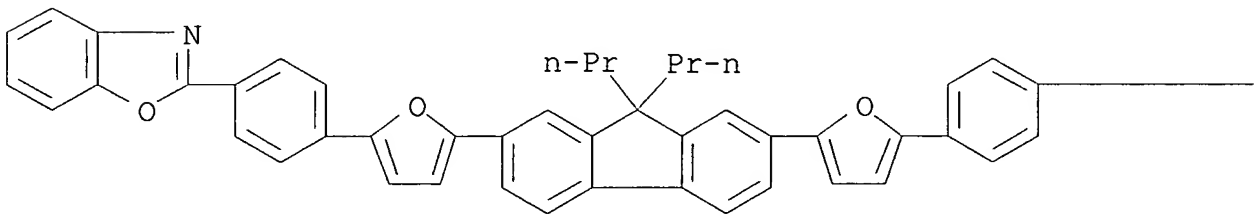
AB Semiempirical computational methods (AM1 for geometries, ZINDO for electronic transition energies) were used to calculate the absorption and fluorescence spectra of oligophenylenes, their heteroarom. substituted derivs., and aryl substituted open-chain and bridged polyenes. The calcns. were calibrated on 61 (for absorption) and 42 (for fluorescence) compds. and reproduced exptl. data with an accuracy of <1200 cm-1. Based on these results, calcns. on possible synthetic targets for compds. to be used as scintillating fluors in high-energy particle detection were performed, whereby absorption and emission wavelengths were predicted for 15 and 34 compds., resp.

IT **256339-23-8**
((E/Z) conformers; quantum chemical calcn. of absorption and fluorescence wavelengths of fluorophores)

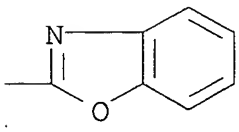
RN 256339-23-8 HCA

CN Benzoxazole, 2,2'-[(9,9-dipropyl-9H-fluorene-2,7-diyl)bis(5,2-furandiyl-4,1-phenylene)]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



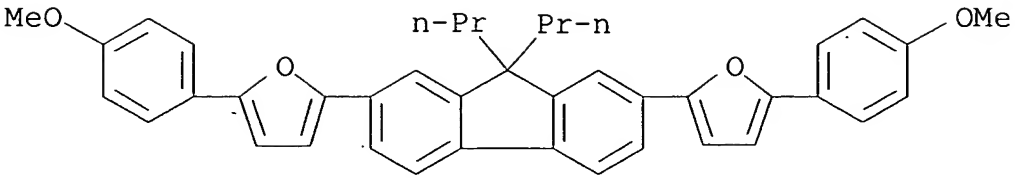
PAGE 1-B



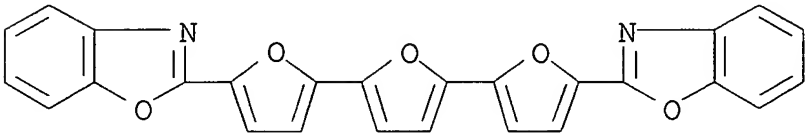
IT **173407-09-5 256339-24-9 256339-25-0**
256339-26-1 256339-27-2 256339-28-3
(quantum chemical calcn. of absorption and fluorescence wavelengths of fluorophores)

RN 173407-09-5 HCA

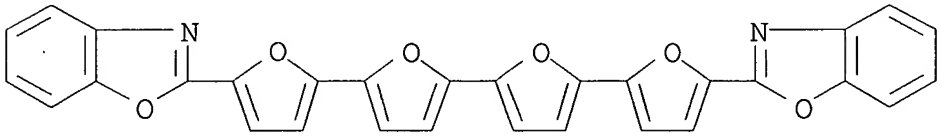
CN Furan, 2,2'-(9,9-dipropyl-9H-fluorene-2,7-diyl)bis[5-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



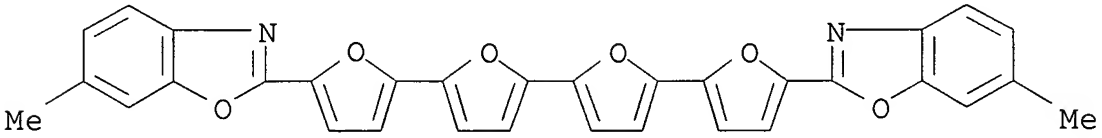
RN 256339-24-9 HCA
CN Benzoxazole, 2,2'-[2,2':5',2''-terfuran]-5,5''-diylbis- (9CI) (CA INDEX NAME)



RN 256339-25-0 HCA
CN Benzoxazole, 2,2'-[2,2':5',2'':5'',2'''-quaterfuran]-5,5'''-diylbis- (9CI) (CA INDEX NAME)

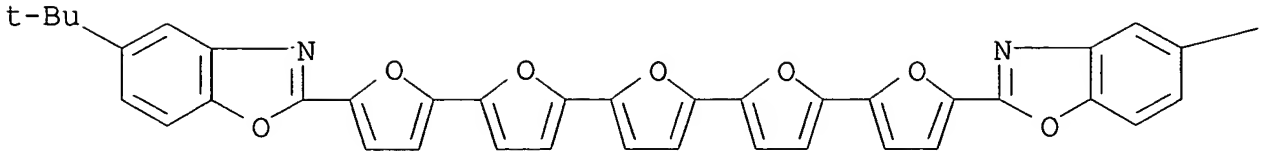


RN 256339-26-1 HCA
CN Benzoxazole, 2,2'-[2,2':5',2'':5'',2'''-quaterfuran]-5,5'''-diylbis[6-methyl- (9CI) (CA INDEX NAME)



RN 256339-27-2 HCA
CN Benzoxazole, 2,2'-[2,2':5',2'':5'',2''':5''',2''''-quinquefuran]-5,5''''-diylbis[5-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

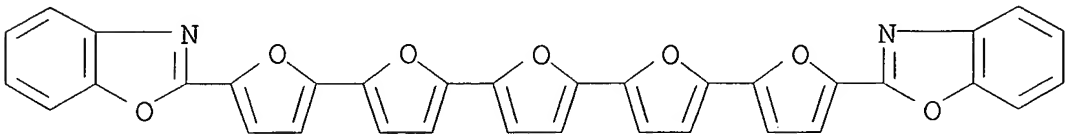
PAGE 1-A



PAGE 1-B

Bu-t

RN 256339-28-3 HCA
CN Benzoxazole, 2,2'-[2,2':5',2'':5'',2''':5''',2''''-quinquefuran]-5,5''''-diylbis- (9CI) (CA INDEX NAME)

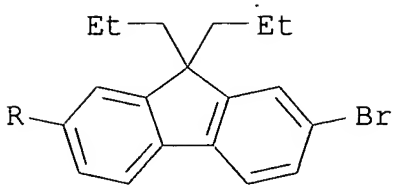


CC 73-1 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 22, 65
IT **256339-23-8** 256339-35-2 256339-36-3
((E/Z) conformers; quantum chemical calcn. of absorption and fluorescence wavelengths of fluorophores)
IT 273-53-0, Benzoxazole 538-81-8 645-49-8, (Z)-1,2-Diphenylethene 833-50-1 904-39-2 1450-63-1 1485-98-9, 1,2-Diphenylcyclopentene 1625-91-8, 4,4'-Di(tert-Butyl)-1,1'-biphenyl 4551-02-4 4982-34-7 5927-01-5 10357-49-0 13021-19-7 13041-66-2 17329-15-6, all-trans-1,6-Diphenyl-1,3,5-hexatriene 17732-30-8 17772-12-2 20235-61-4 21113-62-2 22828-29-1, all-trans-1,8-Diphenyl-1,3,5,7-octatetraene 23125-14-6 23986-41-6 36298-98-3 36416-11-2 36479-34-2 41317-87-7, 1,2-Diphenylcyclohexene 58775-05-6, 2,7-Di(tert-Butyl)fluorene 72033-82-0 84131-40-8 92013-67-7 96581-95-2 104700-13-2 112026-74-1, 9,9-Dipropylfluorene 118593-52-5 118593-53-6 118593-55-8 121368-26-1 133938-43-9 133938-44-0 133949-71-0 144760-02-1 156197-99-8 160751-51-9 173406-92-3 173406-93-4, 2,7-Dicyano-9,9-dipropylfluorene 173406-94-5 173406-95-6 173407-08-4 **173407-09-5** 205884-59-9 220389-46-8 **256339-24-9** **256339-25-0** **256339-26-1** **256339-27-2** **256339-28-3** 256339-29-4

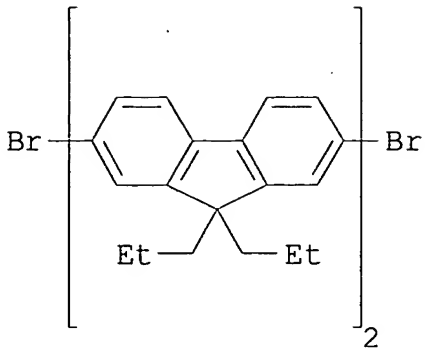
256339-30-7 256339-31-8 256339-32-9 256339-33-0 256339-34-1
256339-37-4 256339-38-5 256339-39-6 256339-40-9 256339-41-0
256339-42-1 256339-43-2 256339-44-3 256339-45-4 256339-46-5
256339-47-6 256339-48-7 256339-49-8 256339-50-1 256339-51-2
256339-52-3 256339-53-4 256339-54-5 256339-55-6
(quantum chemical calcn. of absorption and fluorescence wavelengths of fluorophores)

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

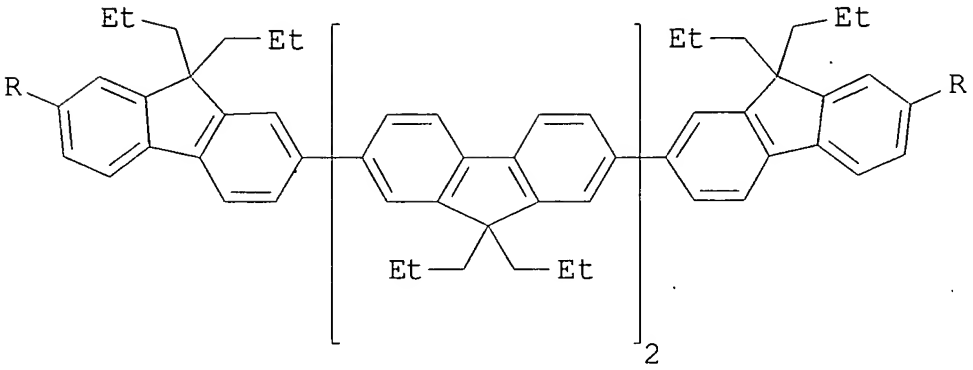
L36 ANSWER 15 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 130:325000 HCA
TITLE: Synthesis of Bridged Oligophenylenes from Fluorene. Part 2.1 Quinquiphenyls to Deciphenyls
AUTHOR(S): Kelley, Charles J.; Ghiorghis, Alem; Qin, Yuanxi; Kauffman, Joel M.; Novinski, John A.; Boyko, Walter J.
CORPORATE SOURCE: Massachusetts College of Pharmacy and Allied Health Sciences, Boston, MA, 02115-5804, USA
SOURCE: Journal of Chemical Research, Synopses (1999), (2), 80-81, 401-418
CODEN: JRPSDC; ISSN: 0308-2342
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:325000
GI



I



II



III

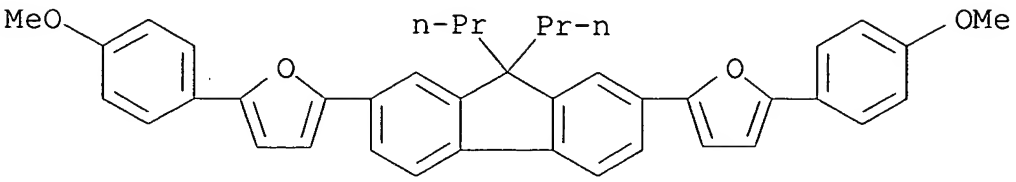
AB Organometallic derivs. of aryl bromides have been coupled with aryl dihalides in the presence of PdCl2(dppb) to produce sym. bridged oligophenylenes that contain five to ten conjugated benzene rings with one to four dialkylmethylene bridges; these products show useful solubility, high quantum efficiency of fluorescence and good photochem. stability. E.g., fluorene I and magnesium are refluxed for 40h in THF; PdCl2[Ph2P(CH2)4PPh2] is added and dibromobifluorene II is extracted form an Ace-Kau apparatus over 2h into the reaction mixture to give bifluorene III in 46% yield as a bridged deciphenyl. These products show useful solubility, high quantum efficiency of fluorescence and good photochem. stability.

IT **173407-09-5P**
(preparation of bridged oligophenylenes by palladium-catalyzed cross coupling of aryl or fluorenyl bromides with aryl Grignard or arylzinc reagents)

RN 173407-09-5 HCA

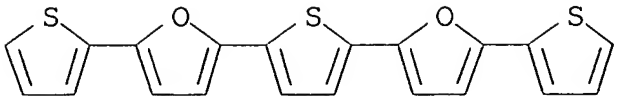
CN Furan, 2,2'-(9,9-dipropyl-9H-fluorene-2,7-diyl)bis[5-(4-

methoxyphenyl)- (9CI) (CA INDEX NAME)

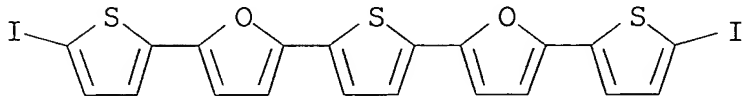


CC 25-28 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 120658-40-4P 131549-47-8P 133358-64-2P 133358-65-3P
153307-02-9P 153307-03-0P 153307-04-1P 153307-06-3P
153307-11-0P 173407-01-7P 173407-02-8P 173407-03-9P
173407-05-1P 173407-06-2P **173407-09-5P** 188652-87-1P
223690-41-3P
(preparation of bridged oligophenylenes by palladium-catalyzed cross
coupling of aryl or fluorenyl bromides with aryl Grignard or arylzinc reagents)
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

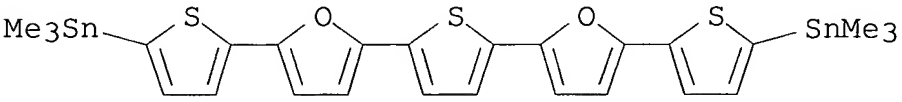
L36 ANSWER 16 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 129:343372 HCA
TITLE: Synthesis of mixed thiophene/furan oligomers by Stille coupling
AUTHOR(S): Hucke, A.; Cava, M. P.
CORPORATE SOURCE: Department of Chemistry, The University of Alabama, Tuscaloosa, AL, 35487-0336, USA
SOURCE: Journal of Organic Chemistry (1998), 63(21), 7413-7417
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:343372
AB A series of mixed thiophene/furan oligomers have been synthesized via organometallic Stille coupling. In some cases, beside cross-coupling products, sym. coupling products were isolated. Oligomers consisting of up to 11 rings were obtained. Attempts to prepare macrocycles with 10 thiophene and furan units were not successful.
IT **157667-21-5**
(preparation of mixed thiophene-furan oligomers by Stille coupling)
RN 157667-21-5 HCA
CN Furan, 2,2'-(2,5-thiophenediyl)bis[5-(2-thienyl)- (9CI) (CA INDEX NAME)



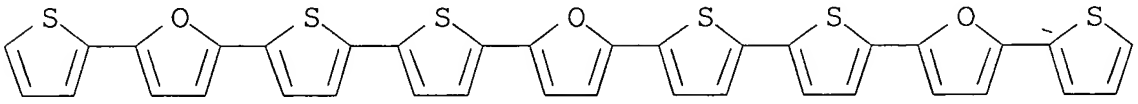
IT **215500-11-1P 215500-16-6P**
(preparation of mixed thiophene-furan oligomers by Stille coupling)
RN 215500-11-1 HCA
CN Furan, 2,2'-(2,5-thiophenediyl)bis[5-(5-iodo-2-thienyl)- (9CI) (CA INDEX NAME)



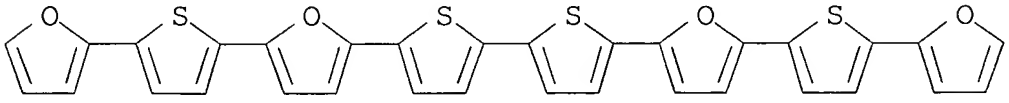
RN 215500-16-6 HCA
CN Stannane, [2,5-thiophenediylbis(5,2-furandiyl-5,2-thiophenediyl)]bis[trimethyl- (9CI) (CA INDEX NAME)



IT **174895-85-3P 215500-14-4P 215500-15-5P**
215500-17-7P 215500-21-3P 215500-22-4P
(preparation of mixed thiophene-furan oligomers by Stille coupling)
RN 174895-85-3 HCA
CN Furan, 2,5-bis[5'-[5-(2-thienyl)-2-furanyl][2,2'-bithiophen]-5-yl]- (9CI) (CA INDEX NAME)

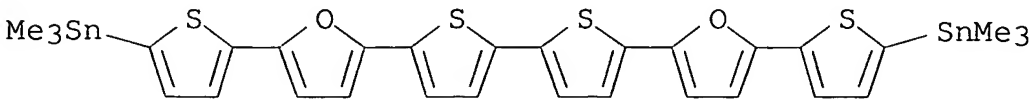


RN 215500-14-4 HCA
CN Furan, 2,2'-[2,2'-bithiophene]-5,5'-diylbis[5-[5-(2-furanyl)-2-thienyl]- (9CI) (CA INDEX NAME)

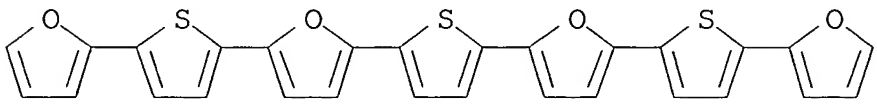


RN 215500-15-5 HCA

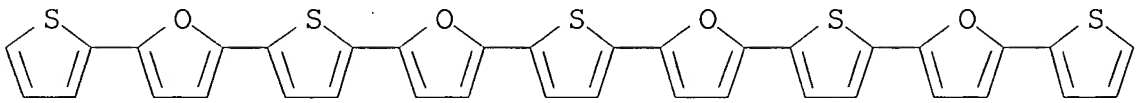
CN Stannane, [[2,2'-bithiophene]-5,5'-diylbis(5,2-furandiyl-5,2-thiophenediyl)]bis[trimethyl- (9CI) (CA INDEX NAME)



RN 215500-17-7 HCA
CN Furan, 2,2'-(2,5-thiophenediyl)bis[5-[5-(2-furanyl)-2-thienyl]- (9CI) (CA INDEX NAME)



RN 215500-21-3 HCA
CN Furan, 2,2'-(2,5-thiophenediyl)bis[5-[5-[5-(2-thienyl)-2-furanyl]-2-thienyl]- (9CI) (CA INDEX NAME)



RN 215500-22-4 HCA
CN Furan, 2,5-bis[5-[5-[5-[5-(2-thienyl)-2-furanyl]-2-thienyl]-2-furanyl]-2-thienyl]- (9CI) (CA INDEX NAME)

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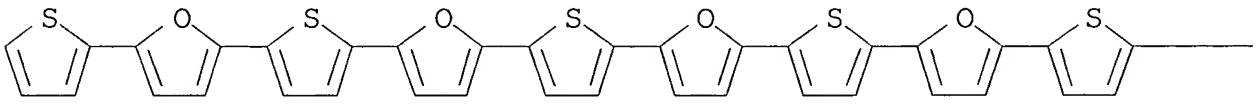

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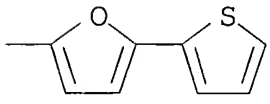


CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
IT 492-97-7, 2,2'-Bithiophene 625-88-7, 2,5-Diiodothiophene

1066-45-1, Trimethyltin chloride 1461-22-9, Tributylstannyl chloride 51583-40-5, 2-(Trimethylstannyl)furan 54829-48-0, 2-Iodofuran 88089-34-3 118486-94-5, 2-(Tributylstannyl)furan **157667-21-5** 215500-19-9 215500-20-2
(preparation of mixed thiophene-furan oligomers by Stille coupling)
IT 1665-29-8P 171290-94-1P 215500-09-7P 215500-10-0P **215500-11-1P** 215500-12-2P 215500-13-3P **215500-16-6P**
(preparation of mixed thiophene-furan oligomers by Stille coupling)
IT **174895-85-3P 215500-14-4P 215500-15-5P** **215500-17-7P** 215500-18-8P **215500-21-3P** **215500-22-4P**
(preparation of mixed thiophene-furan oligomers by Stille coupling)
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

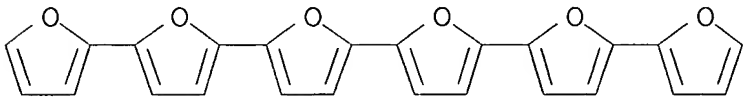
L36 ANSWER 17 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 124:246135 HCA
TITLE: Organic superlattice material, production thereof and device therefrom
INVENTOR(S): Hamano, Koji; Kurata, Tetsuyuki; Fuchigami, Hiroyuki; Nobutoki, Eiji; Fukada, Che; Nakao, Yukyasu
PATENT ASSIGNEE(S): Mitsubishi Electric Corp, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07325329	A2	19951212	JP 1994-120058	19940601
JP 2975530	B2	19991110		
PRIORITY APPLN. INFO.:			JP 1994-120058	19940601

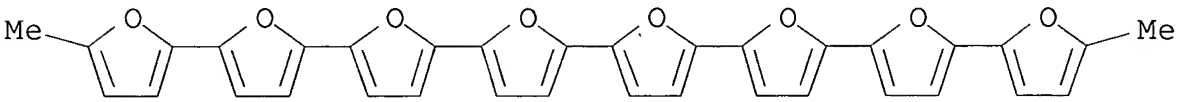
AB An organic material, suitable for use as nonlinear optical and electronic materials, is prepared by laminating ≥2 kind of organic thin films having a thickness 0.5-100 nm, wherein the organic thin film comprises π-conjugated linear oligomers.

IT **174895-49-9 174895-51-3 174895-53-5**
174895-55-7 174895-57-9 174895-59-1
174895-61-5 174895-67-1 174895-69-3
174895-73-9 174895-79-5 174895-85-3
174895-86-4 174895-93-3 174895-95-5
174896-05-0 174896-06-1 174896-07-2
174896-08-3 174896-15-2 174896-16-3
174896-21-0 174896-26-5 174896-32-3
174896-36-7 174896-38-9 174896-43-6
(organic superlattice material, production thereof and device therefrom)

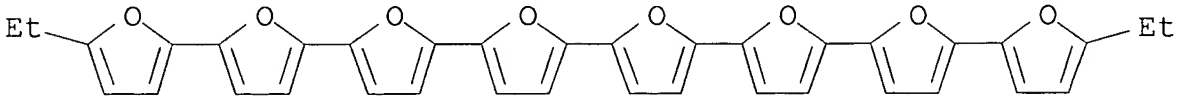
RN 174895-49-9 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2''''':5''''',2'''''-Sexifuran (9CI) (CA INDEX NAME)



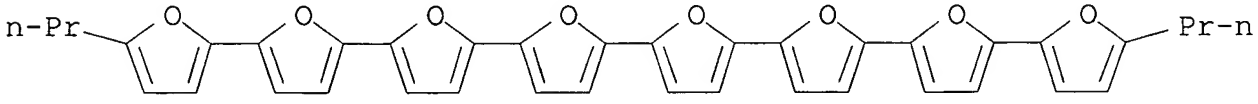
RN 174895-51-3 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2''''':5''''',2'''''':5''''''', 2'''''''-Octifuran, 5,5'''''''-dimethyl- (9CI) (CA INDEX NAME)



RN 174895-53-5 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2''''':5''''',2'''''':5''''''', 2'''''''-Octifuran, 5,5'''''''-diethyl- (9CI) (CA INDEX NAME)

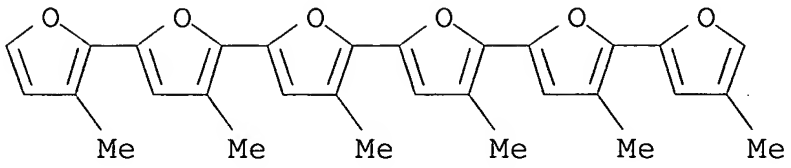


RN 174895-55-7 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2''''':5''''',2'''''':5''''''', 2'''''''-Octifuran, 5,5'''''''''-dipropyl- (9CI) (CA INDEX NAME)

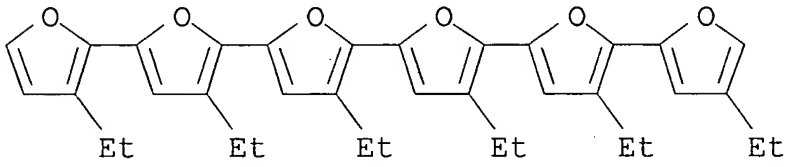


RN 174895-57-9 HCA

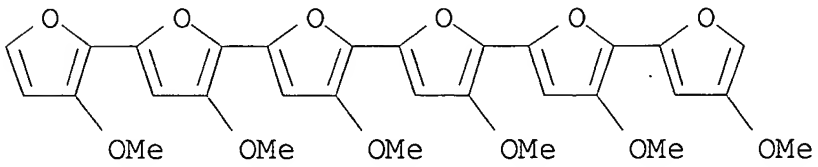
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2'''''-Sexifuran, 3',3'',3''',3'''',3''''',4-hexamethyl- (9CI) (CA INDEX NAME)



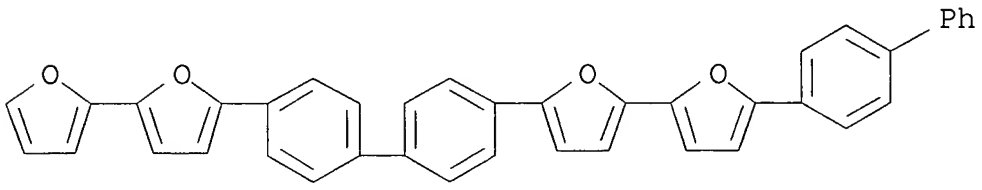
RN 174895-59-1 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2'''''-Sexifuran, 3',3'',3''',3'''',3''''',4-hexaethyl- (9CI) (CA INDEX NAME)



RN 174895-61-5 HCA
CN 2,2':5',2'':5'',2''':5''',2'''':5'''',2'''''-Sexifuran, 3',3'',3''',3'''',3''''',4-hexamethoxy- (9CI) (CA INDEX NAME)



RN 174895-67-1 HCA
CN 2,2'-Bifuran, 5-(4'-[2,2'-bifuran]-5-yl[1,1'-biphenyl]-4-yl)-5'-[1,1'-biphenyl]-4-yl- (9CI) (CA INDEX NAME)



RN 174895-69-3 HCA
CN 2,2':5',2''-Terfuran, 5-methyl-5''-[4'-[5''-(4'-methyl[1,1'-biphenyl]-4-yl)[2,2':5',2''-terfuran]-2-yl][1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

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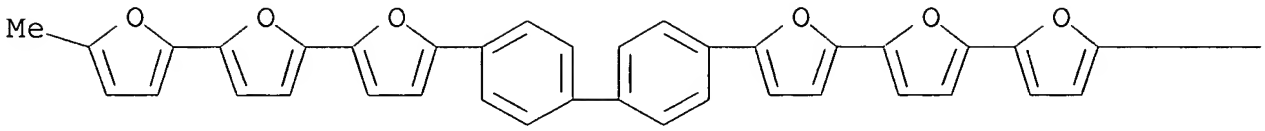

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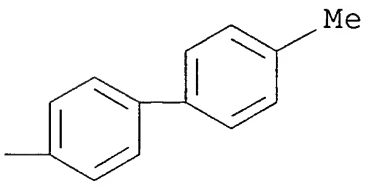
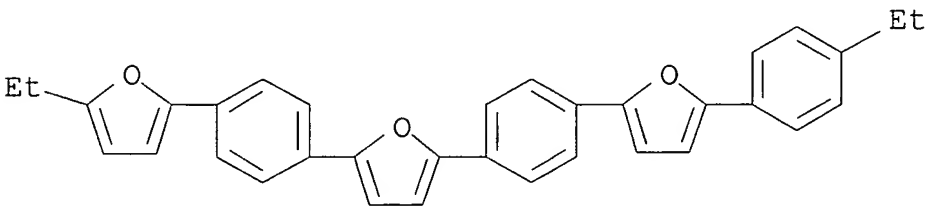
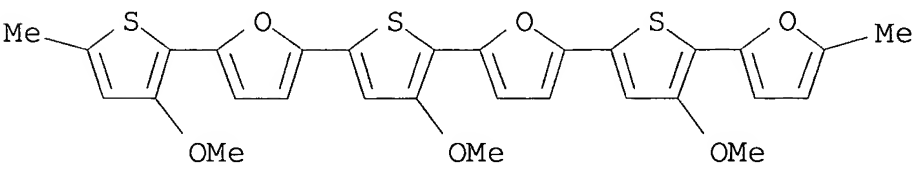


RN 174895-73-9 HCA
CN Furan, 2-[4-(5-ethyl-2-furanyl)phenyl]-5-[4-[5-(4-ethylphenyl)-2-furanyl]phenyl]- (9CI) (CA INDEX NAME)

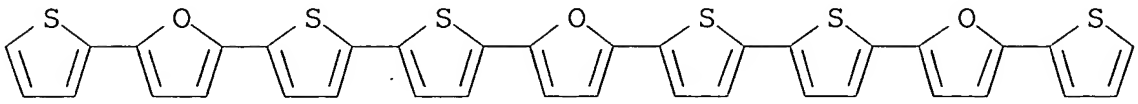


RN 174895-79-5 HCA
CN Furan, 2-[3-methoxy-5-[5-(3-methoxy-5-methyl-2-thienyl)-2-furanyl]-2-thienyl]-5-[4-methoxy-5-(5-methyl-2-furanyl)-2-thienyl]- (9CI) (CA INDEX NAME)

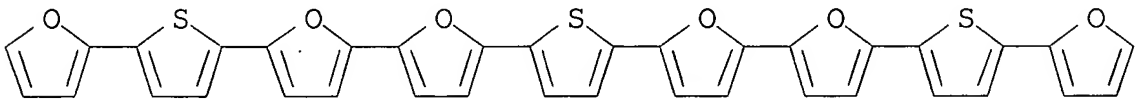


RN 174895-85-3 HCA

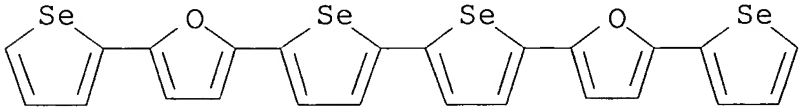
CN Furan, 2,5-bis[5'-[5-(2-thienyl)-2-furanyl][2,2'-bithiophen]-5-yl]- (9CI) (CA INDEX NAME)



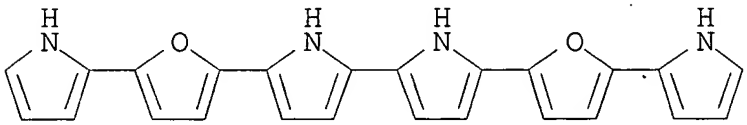
RN 174895-86-4 HCA
CN 2,2'-Bifuran, 5,5''-(2,5-thiophenediyl)bis[5'-[5-(2-furanyl)-2-thienyl]- (9CI) (CA INDEX NAME)



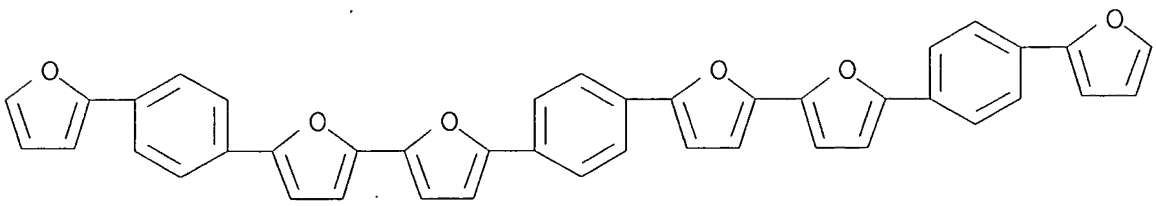
RN 174895-93-3 HCA
CN Furan, 2,2'-[2,2'-biselenophene]-5,5'-diylbis[5-selenophene-2-yl- (9CI) (CA INDEX NAME)



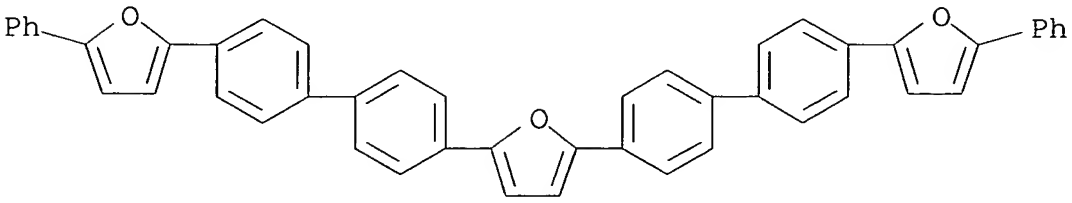
RN 174895-95-5 HCA
CN 2,2'-Bi-1H-pyrrole, 5,5'-bis[5-(1H-pyrrol-2-yl)-2-furanyl]- (9CI) (CA INDEX NAME)



RN 174896-05-0 HCA
CN 2,2'-Bifuran, 5,5''-(1,4-phenylene)bis[5'-[4-(2-furanyl)phenyl]- (9CI) (CA INDEX NAME)

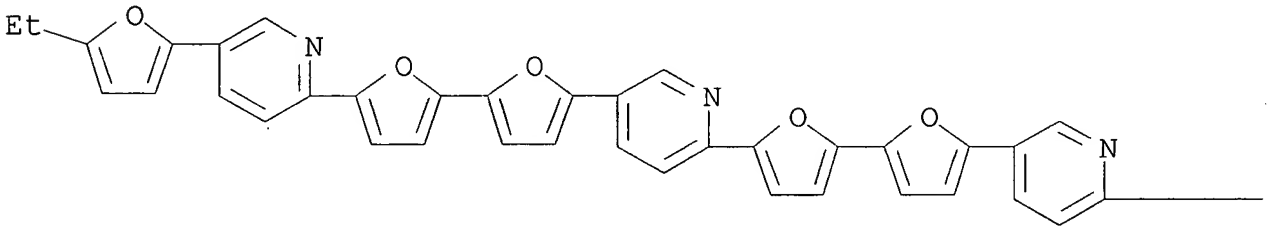


RN 174896-06-1 HCA
CN Furan, 2,5-bis[4'-(5-phenyl-2-furanyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

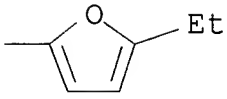


RN 174896-07-2 HCA
CN Pyridine, 5-[5'-[5-(5-ethyl-2-furanyl)-2-pyridinyl][2,2'-bifuran]-5-yl]-2-[5'-[6-(5-ethyl-2-furanyl)-3-pyridinyl][2,2'-bifuran]-5-yl]- (9CI) (CA INDEX NAME)

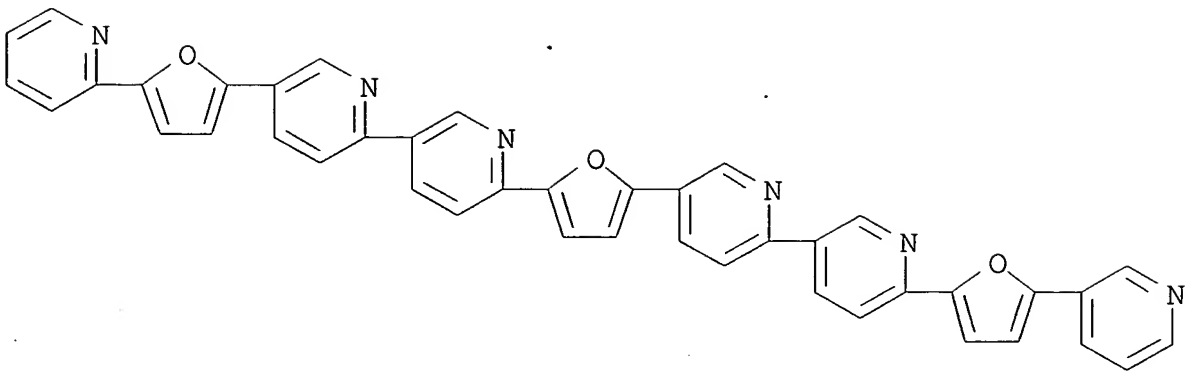
PAGE 1-A



PAGE 1-B

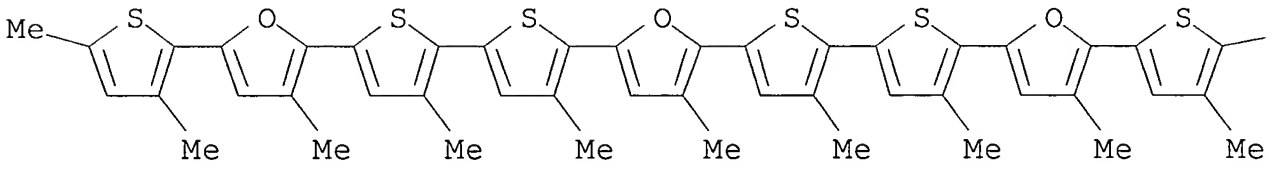


RN 174896-08-3 HCA
CN 2,3'-Bipyridine, 5-[5-(2-pyridinyl)-2-furanyl]-6'-[5-[6'-[5-(3-pyridinyl)-2-furanyl][2,3'-bipyridin]-5-yl]-2-furanyl]- (9CI) (CA INDEX NAME)



RN 174896-15-2 HCA
CN Furan, 5-[5'-[5-(3,5-dimethyl-2-thienyl)-3-methyl-2-furanyl]-3',4-dimethyl[2,2'-bithiophen]-5-yl]-2-[5'-[5-(4,5-dimethyl-2-thienyl)-4-methyl-2-furanyl]-3,4'-dimethyl[2,2'-bithiophen]-5-yl]-3-methyl- (9CI) (CA INDEX NAME)

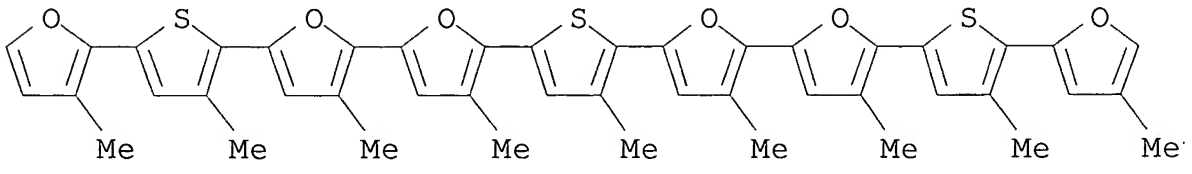
PAGE 1-A



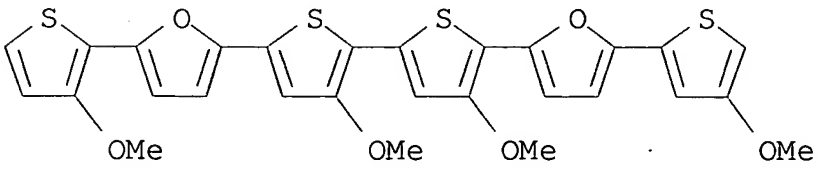
PAGE 1-B

—Me

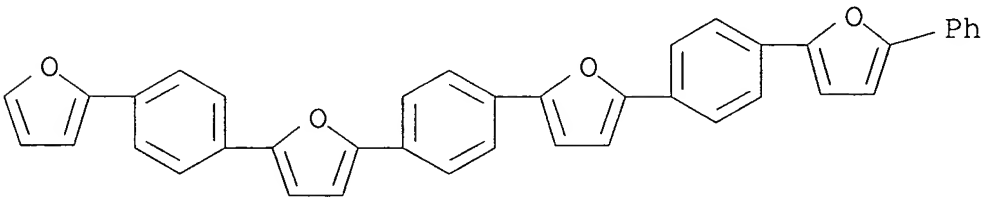
RN 174896-16-3 HCA
CN 2,2'-Bifuran, 5-[5-[3',4-dimethyl-5'-[3-methyl-5-(3-methyl-2-furanyl)-2-thienyl][2,2'-bifuran]-5-yl]-3-methyl-2-thienyl]-3,4'-dimethyl-5'-[4-methyl-5-(4-methyl-2-furanyl)-2-thienyl]- (9CI) (CA INDEX NAME)



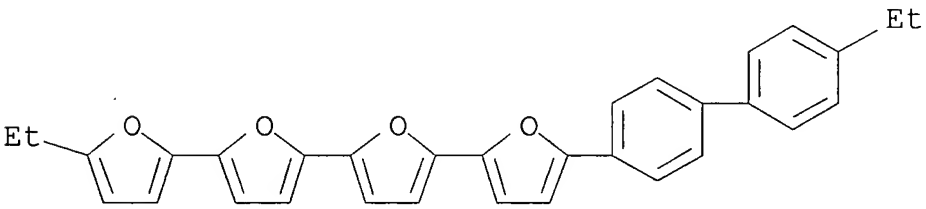
RN 174896-21-0 HCA
CN Furan, 2-[3,4'-dimethoxy-5'-[5-(4-methoxy-2-thienyl)-2-furanyl][2,2'-bithiophen]-5-yl]-5-(3-methoxy-2-thienyl)- (9CI) (CA INDEX NAME)



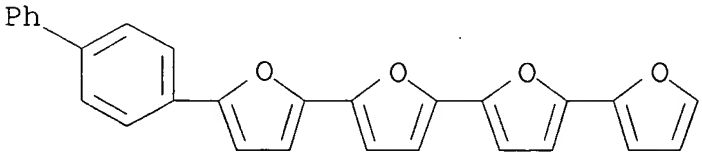
RN 174896-26-5 HCA
CN Furan, 2-[4-[5-[4-(2-furanyl)phenyl]-2-furanyl]phenyl]-5-[4-(5-phenyl-2-furanyl)phenyl]- (9CI) (CA INDEX NAME)



RN 174896-32-3 HCA
CN 2,2':5',2'':5'',2'''-Quaterfuran, 5-ethyl-5'''-(4'-ethyl[1,1'-biphenyl]-4-yl)- (9CI) (CA INDEX NAME)

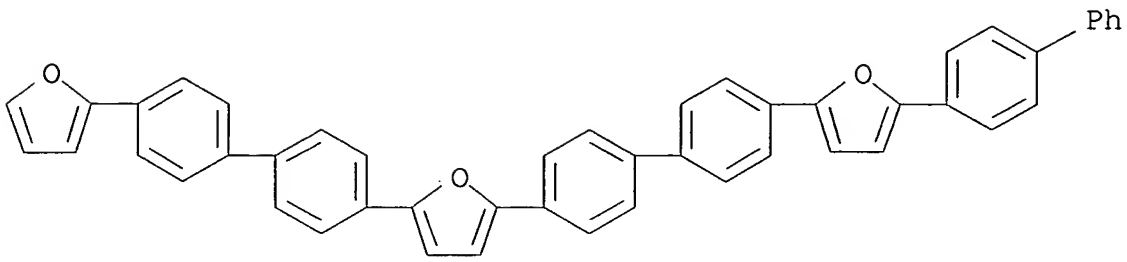


RN 174896-36-7 HCA
CN 2,2':5',2'':5'',2'''-Quaterfuran, 5-[1,1'-biphenyl]-4-yl- (9CI) (CA INDEX NAME)

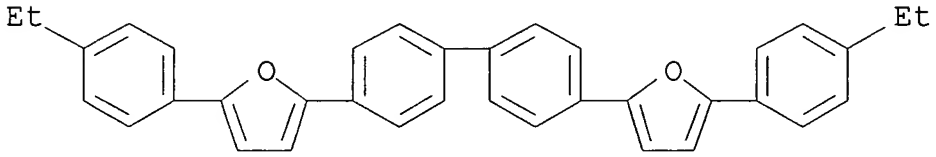


RN 174896-38-9 HCA
CN Furan, 2-[4'-(5-[1,1'-biphenyl]-4-yl-2-furanyl)[1,1'-biphenyl]-4-yl]-

5-[4'-(2-furanyl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 174896-43-6 HCA
CN Furan, 2,2'-[1,1'-biphenyl]-4,4'-diylbis[5-(4-ethylphenyl)- (9CI) (CA INDEX NAME)



IC ICM G02F001-35
ICS C08F034-00; C08F034-04; C09K009-02
ICA C09K003-00
CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 75, 76
IT 4499-83-6 21850-31-7 60602-70-2 70352-21-5 86100-63-2
88493-55-4 102192-98-3 108664-05-7 147237-94-3 147237-95-4
151629-36-6 174895-33-1 174895-34-2 174895-35-3 174895-36-4
174895-37-5 174895-38-6 174895-39-7 174895-40-0 174895-41-1
174895-42-2 174895-43-3 174895-44-4 174895-45-5 174895-46-6
174895-47-7 174895-48-8 **174895-49-9** 174895-50-2
174895-51-3 174895-52-4 **174895-53-5**
174895-54-6 **174895-55-7** 174895-56-8 **174895-57-9**
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174895-70-6 174895-71-7 174895-72-8 **174895-73-9**
174895-74-0 174895-75-1 174895-76-2 174895-77-3 174895-78-4
174895-79-5 174895-80-8 174895-81-9 174895-82-0
174895-83-1 174895-84-2 **174895-85-3** **174895-86-4**
174895-87-5 174895-88-6 174895-89-7 174895-90-0 174895-91-1
174895-92-2 **174895-93-3** 174895-94-4 **174895-95-5**
174895-96-6 174895-97-7 174895-98-8 174895-99-9 174896-00-5
174896-01-6 174896-02-7 174896-03-8 174896-04-9

174896-05-0 **174896-06-1** **174896-07-2**
174896-08-3 174896-09-4 174896-10-7 174896-11-8
174896-12-9 174896-13-0 174896-14-1 **174896-15-2**
174896-16-3 174896-17-4 174896-18-5 174896-19-6
174896-20-9 **174896-21-0** 174896-22-1 174896-23-2
174896-24-3 174896-25-4 **174896-26-5** 174896-27-6
174896-28-7 174896-29-8 174896-30-1 174896-31-2
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174896-36-7 174896-37-8 **174896-38-9**
174896-39-0 174896-40-3 174896-41-4 174896-42-5
174896-43-6 174896-44-7 174896-45-8 174896-46-9
174896-47-0
(organic superlattice material, production thereof and device therefrom)

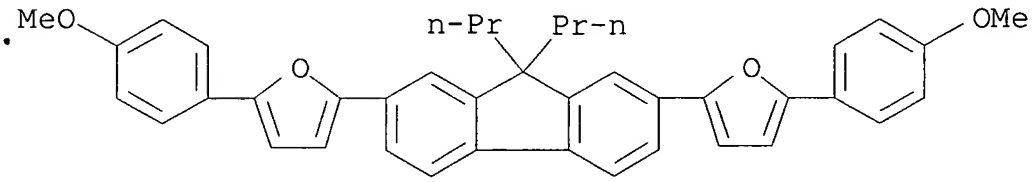
L36 ANSWER 18 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 124:158852 HCA
TITLE: Electronic absorption and emission spectral data and fluorescence quantum yields of bridged p-oligophenylenes, bi- to deciphenyls, and related furans and carbazoles
AUTHOR(S): Kauffman, Joel M.; Litak, Peter T.; Novinski, John A.; Kelley, Charles J.; Ghiorghis, Alem; Qin, Yuanxi
CORPORATE SOURCE: Department of Chemistry, Philadelphia College of Pharmacy & Science, Philadelphia, 19104-4495, USA
SOURCE: Journal of Fluorescence (1995), 5(3), 295-305
CODEN: JOFLEN; ISSN: 1053-0509
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Absorption and fluorescence emission spectral data, as well as fluorescence quantum yields (Φf), were determined for 41 p-oligophenylene compds. containing 2-6, 8, and 10 benzene rings. Of 29 compds. containing carbon-bridged rings (fluorenes), 28 were dialkylated on each bridge for improved solubility and photostability. Absorption maximum for oligophenylenes were observed at wavelengths as long as 366 nm, emission maximum to 437 nm, and molar extinction coeffs. (ε) as large as 153,000 L/mol-cm; all three exceeded predicted maximum values for the corresponding unbridged oligophenylenes. The substitution of furan for benzene or carbazole for a fluorene (two examples each) bathochromically shifted absorption and emission maximum Dialkylated carbon bridges bathochromically shifted absorption and emission maximum, and lowered

Φf in biphenyl and in one terphenyl analog, but appeared to cause no diminution of Φf in higher oligophenylenes. Bis(2-methoxyethyl) substitution on the bridges, incorporated to provide solubility in polar solvents, lowered Φf in all examples. Tertiary alkyl substituents on terminal rings bathochromically shifted the absorption and emission maximum and generally increased Φf. The "loose bolt" effect, which lowers Φf in mononuclear substituted benzenes, may operate in 9,9-dialkylfluorenes, but not in 2,7-di-tert-butylfluorene or in higher oligophenylenes. Cyclic ether and methoxy substituents as auxofluors on terminal rings generally bathochromically shifted absorption and emission maximum and increased ε and Φf. Cyano substituents bathochromically shifted absorption and emission maximum, and increased ε, but lowered Φf slightly.

IT **173407-09-5**
(photophys. properties of oligophenylene fluors)

RN 173407-09-5 HCA

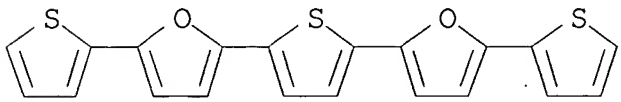
CN Furan, 2,2'-(9,9-dipropyl-9H-fluorene-2,7-diyl)bis[5-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



CC 73-1 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 74

IT 1625-91-8, 4,4'-Di-tert-butylbiphenyl 13021-19-7, 4,4''-Dimethoxyterphenyl 13041-66-2, 4-Methoxyterphenyl 58775-05-6, 2,7-Di-tert-butylfluorene 104700-13-2, 3,5,3'',5''-Tetra-tert-butyl-p-terphenyl 112026-74-1, 9,9-Dipropylfluorene 118593-52-5 118593-53-6 118593-55-8 120658-40-4 121368-26-1, 4-Cyano-4''-methoxyterphenyl 121838-04-8, 4,4''-Di-tert-amyl-p-terphenyl 131549-47-8 131549-48-9 133358-63-1 133358-64-2 133938-43-9, 4-tert-Amyl-p-terphenyl 133938-44-0, 4-Fluoro-4''-methoxyterphenyl 133949-71-0, 2-(4-Methoxyphenyl)-9,9-dipropylfluorene 153307-02-9 153307-03-0 153307-06-3 153307-11-0 173406-92-3, 2-Cyano-9-ethylcarbazole 173406-93-4, 2,7-Dicyano-9,9-dipropylfluorene 173406-94-5, 2-(4-tert-Butylphenyl)-9,9-dipropylfluorene 173406-95-6, 9-Ethyl-2-(4-methoxyphenyl)carbazole 173406-96-7 173406-97-8 173406-98-9 173406-99-0 173407-00-6 173407-01-7 173407-02-8 173407-03-9 173407-05-1 173407-06-2 173407-07-3 173407-08-4 **173407-09-5** 188652-87-1
(photophys. properties of oligophenylene fluors)

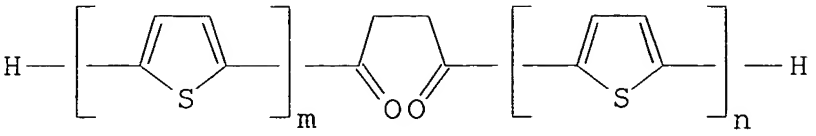
L36 ANSWER 19 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 122:213883 HCA
TITLE: Furan- and pyrrole-containing analogs of α-quinquethiophene: spectroscopic and electrochemical properties
AUTHOR(S): Parakka, James P.; Cava, Michael P.
CORPORATE SOURCE: Department of Chemistry, University of Alabama, Box 870336, Tuscaloosa, AL, 35487-0336, USA
SOURCE: Synthetic Metals (1995), 68(3), 275-9
CODEN: SYMEDZ; ISSN: 0379-6779
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of pentacyclic analogs of α-quinquethiophene containing one or two furan or pyrrole units has been synthesized. The synthesis is based on the cyanide-catalyzed Stetter reaction, providing the ketonic precursors to the pentacycles. Spectral and electrochem. investigations show that the redox-stable mixed pentacycles display hypsochromic shifts in their absorption maxima, as well as a greater ease of oxidation, in comparison to α-quinquethiophene.
IT **157667-21-5P**
(preparation, spectrochem., and electrochem. of furan- and pyrrole-containing α-quinquethiophene analogs)
RN 157667-21-5 HCA
CN Furan, 2,2'-(2,5-thiophenediyl)bis[5-(2-thienyl)- (9CI) (CA INDEX NAME)



CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
IT 5660-45-7P 155042-09-4P 157667-20-4P **157667-21-5P** 161869-63-2P 161869-64-3P 161869-65-4P
(preparation, spectrochem., and electrochem. of furan- and pyrrole-containing α-quinquethiophene analogs)

L36 ANSWER 20 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 121:179431 HCA
TITLE: Synthesis of furan- and pyrrole-containing α-oligothiophenes via 1,4-diketones
AUTHOR(S): Chen, Liang-Huei; Wang, Chin-Yu; Luo, Thung-Mei H.
CORPORATE SOURCE: Dep. Appl. Chem., Chia Nan Junior Coll. Pharm., Tainan, 71710, Taiwan

SOURCE: Heterocycles (1994), 38(6), 1393-8
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI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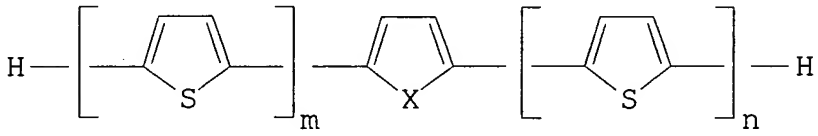
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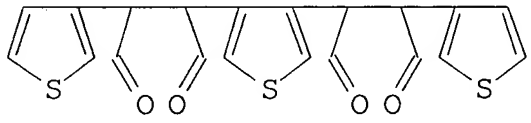
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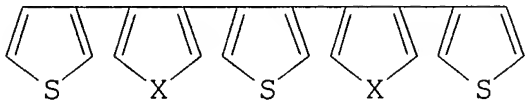
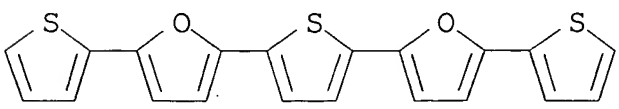

IV

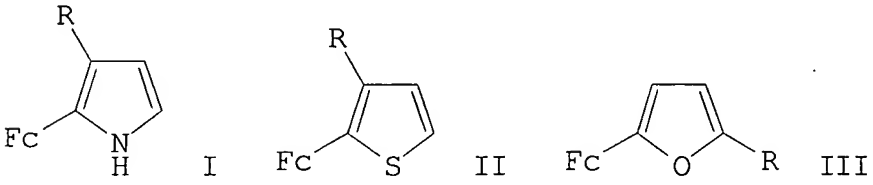
AB Cyclization of the 1,4-dithienyl-1,4-diketones I (m, n = 1, 2) by acid catalyst furnished the α-thienylfurans II (X = O), whereas condensation with ammonium acetate provided the α-thienylpyrroles II (X = NH). The 2,5-bis[4-(2-thienyl)-1,4-butanedionyl]thiophene (III) similarly gave the first synthesis of 2,5-bis[2-(5,2'-thienyl)pyrryl]thiophene (IV, = NH) and 2,5-bis[2-(5,2'-thienyl)furyl]thiophenes (IV, = O).

IT **157667-21-5P**
(preparation of)
RN 157667-21-5 HCA
CN Furan, 2,2'-(2,5-thiophenediyl)bis[5-(2-thienyl)- (9CI) (CA INDEX NAME)

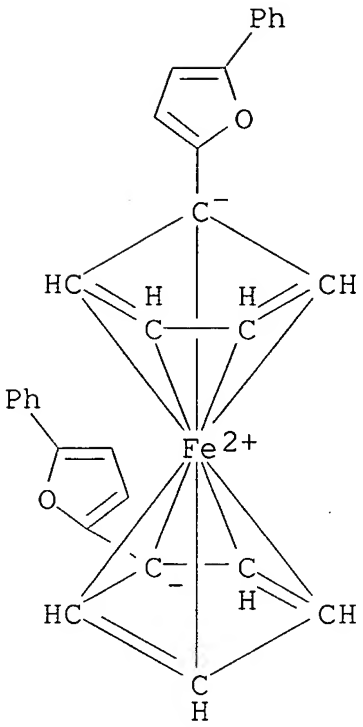


CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
IT 88089-34-3P 89814-62-0P 157667-16-8P 157667-17-9P
157667-18-0P 157667-19-1P 157667-20-4P **157667-21-5P**
(preparation of)

L36 ANSWER 21 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 120:270724 HCA
TITLE: Synthesis of ferrocenyl-substituted heterocycles: the beneficial effect of the microwave irradiation
AUTHOR(S): Puciova, Monika; Ertl, Peter; Toma, Stefan
CORPORATE SOURCE: Dep. Org. Chem., Comenius Univ., Bratislava, 84215, Slovakia
SOURCE: Collection of Czechoslovak Chemical Communications (1994), 59(1), 175-85
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:270724
GI



AB The synthesis of ferrocenyl-substituted thiophenes, furans, pyrroles, pyrimidine and pyrazole has been studied. 2-Ferrocenylpyrroles I (R = H, Ph, Fc = ferrocenyl) were prepared from ferrocenyl ketoximes FcC(CH2R):NOH and acetylene in DMSO-KOH mixture, whereas 3-chloro-3-ferrocenylacrylaldehydes and thioglycolic or glycolic acids were the starting materials for the synthesis of the thiophene and furan derivs., e.g., II and III, resp. The yields were significantly enhanced when the reactions were carried out in a microwave oven. The lower stability of 2-ferrocenylfuran in comparison with 2-ferrocenylthiophene is discussed on the basis of semiempirical quantum chemical calcns.
IT **154671-98-4P**
(preparation of)
RN 154671-98-4 HCA
CN Ferrocene, 1,1'-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



CC 29-12 (Organometallic and Organometalloidal Compounds)
IT 1291-56-1P 1291-62-9P 97316-82-0P 117153-80-7P 144547-16-0P
144547-17-1P 154671-96-2P **154671-98-4P** 154671-99-5P
154672-00-1P 154672-02-3P 154672-03-4P 154672-04-5P
154718-46-4P 154718-47-5P
(preparation of)

L36 ANSWER 22 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 117:70520 HCA
TITLE: Tetracarboxylic acid dianhydrides
INVENTOR(S): Okada, Koji
PATENT ASSIGNEE(S): Kanegafuchi Kagaku Kogyo K. K., Japan
SOURCE: Eur. Pat. Appl., 14 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 477539	A1	19920401	EP 1991-114177	

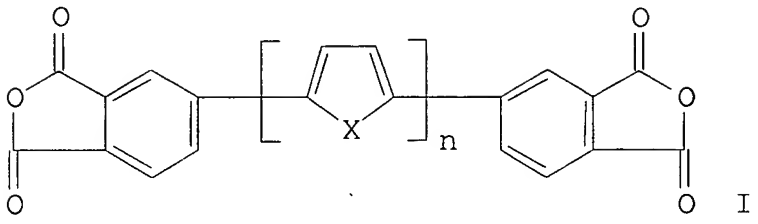
				199108 23
EP 477539	B1	19951108		
R: BE, DE, FR, GB				
JP 04103582	A2	19920406	JP 1990-223363	199008 24
JP 2933695	B2	19990816		
JP 04103579	A2	19920406	JP 1990-223364	199008 24
JP 2876537	B2	19990331		
US 5122617	A	19920616	US 1991-749342	199108 23

PRIORITY APPLN. INFO.: JP 1990-223363 A 199008 24

JP 1990-223364 A 199008 24

OTHER SOURCE(S): MARPAT 117:70520

GI



I

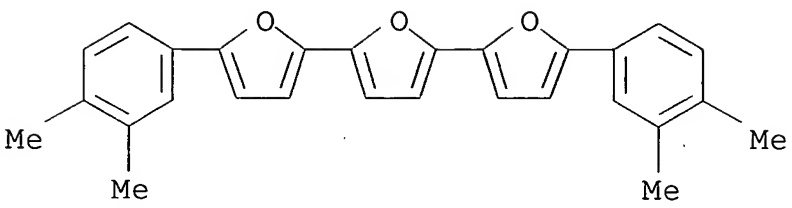
AB The dianhydrides I (X = O, S; n = 1-3) are useful in preparation of polyimides with low thermal expansion, low dielec. constant, and low hydroscopicity. Bis(3-phthalic anhydrido)thienyl (II) was prepared by oxidation of a 2,5-bis(3-o-xylino)thienyl-3-iodo-o-xylene reaction product. A copolymer of II and p-phenylenediamine had thermal expansion coefficient 1.2 + 10-3 °C-1, dielec. constant 2.7, and water absorption 0.5%.

IT **142647-76-5P**
(preparation and oxidation of)

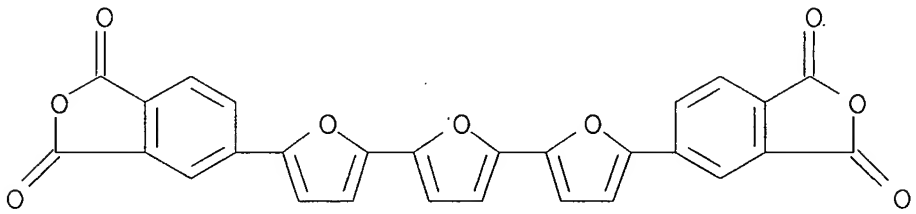
RN 142647-76-5 HCA

CN 2,2':5',2''-Terfuran, 5,5''-bis(3,4-dimethylphenyl)- (9CI) (CA

INDEX NAME)



IT **142628-87-3P**
(preparation and polymerization of)
RN 142628-87-3 HCA
CN 1,3-Isobenzofurandione, 5,5'-[2,2':5',2''-terfuran]-5,5''-diylbis- (9CI) (CA INDEX NAME)



IC ICM C07D409-14
ICS C07D307-89
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27
IT 94580-33-3P 142628-78-2P 142628-80-6P 142628-82-8P
142647-76-5P 143375-80-8P
(preparation and oxidation of)
IT 142628-79-3P 142628-81-7P 142628-83-9P 142628-84-0P
142628-86-2P **142628-87-3P**
(preparation and polymerization of)

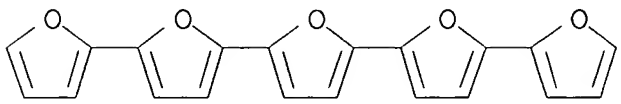
L36 ANSWER 23 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 115:265264 HCA
TITLE: Determination of the electronic structure of oligofurans and extrapolation to polyfuran
AUTHOR(S): Distefano, Giuseppe; Jones, Derek; Guerra, Maurizio; Favaretto, Laura; Modelli, Alberto; Mengoli, Giuliano
CORPORATE SOURCE: Dip. Chim., Univ. Ferrara, Ferrara, 44100, Italy
SOURCE: Journal of Physical Chemistry (1991), 95(24), 9746-53
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Gas-phase ionization and attachment energy values of the first few oligomers of furan were determined exptl. and by semiempirical calcns. and extrapolated to polyfuran. A comparison with the corresponding data determined previously for thiophene analogs indicates that (ideal, gas-phase) polyfuran should behave like polythiophene toward p doping and show a lesser disposition toward n doping. Cyclic voltammetry data show that in solution the oxidation of furan derivs. occurs as easily as for the thiophene analogs, whereas reduction is slightly more difficult. MINDO/3 valence ionization and electron affinity values for a quinoid form derived from the trimers indicate that furan and 5thiophene derivs. have similar electronic structures. It appears, therefore, that the low values of elec. conductivity reported for p-doped polyfuran are likely due to solid-state disorder.

IT **137040-24-5**
(electronic structure of)

RN 137040-24-5 HCA

CN 2,2':5',2'':5'',2''':5''',2''''-Quinquefuran (9CI) (CA INDEX NAME)



CC 72-2 (Electrochemistry)
Section cross-reference(s): 22, 27, 36, 65

IT 110-00-9, Furan **137040-24-5**
(electronic structure of)

L36 ANSWER 24 OF 35 HCA COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 114:179908 HCA

TITLE: Inhibition of mitochondrial respiration by neutral, monocationic, and dicationic bispyridines related to the dopaminergic neurotoxin 1-methyl-4-phenylpyridinium cation (MPP+)

AUTHOR(S): Singh, Malvinder P.; Wang, Fengjiang; Hoppel, Charles L.; Sayre, Lawrence M.

CORPORATE SOURCE: Dep. Chem., Case West. Reserve Univ., Cleveland, OH, 44106, USA

SOURCE: Archives of Biochemistry and Biophysics (1991), 286(1), 138-46
CODEN: ABBIA4; ISSN: 0003-9861

DOCUMENT TYPE: Journal

LANGUAGE: English

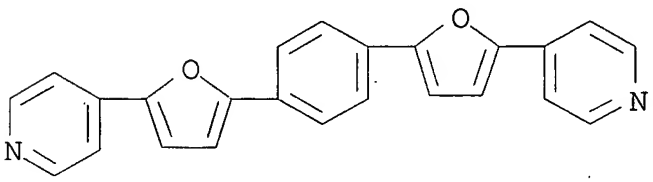
AB The cytotoxic effect of the dopaminergic neurotoxin MPP+ is believed

to be associated with a compromise in cellular energy arising as a consequence of its persistent inhibition of mitochondrial respiration. MPP+ is a rather weak inhibitor of electron transport, but it undergoes passive accumulation inside actively respiring mitochondria in response to the transmembrane electrochem. potential gradient. To test the prediction that dicationic analogs of MPP+ might be concentrated to a much greater extent and thereby exert especially potent inhibition of respiration on the intact organelle, four differently spaced bispyridines, each in neutral, monocationic, and dicationic forms were evaluated for their inhibitory activities in intact mitochondria and in electron transport particles (ETP). Compared to the neutrals, the monocations, and especially the dications exhibit reduced inhibition in ETP, but the inhibition in mitochondria is enhanced selectively for the cationic inhibitors presumably on account of their accumulation in the mitochondrial matrix. This enhancement is limited by the relatively poor ability of the cationic bispyridines to enter mitochondria, as judged from expts. which evaluated the rate of onset of inhibition (without preincubation), in the absence and presence of tetraphenylborate. The dications appear to be transported less well than the monocations, and only the most lipophilic dication exhibited a substantially greater accumulation-dependent enhancement of inhibitory activity on mitochondria than did the corresponding monocation. The compds. studied here constitute a novel class of respiratory chain probes which may be useful for a variety of studies on mitochondria.

IT **133416-08-7 133416-09-8 133416-10-1**
(electron transport and respiration by heart and liver mitochondria response to)

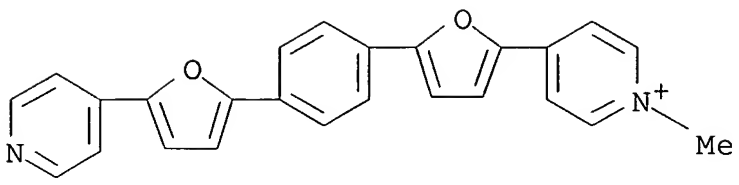
RN 133416-08-7 HCA

CN Pyridine, 4,4'-(1,4-phenylenedi-5,2-furandiyl)bis- (9CI) (CA INDEX NAME)



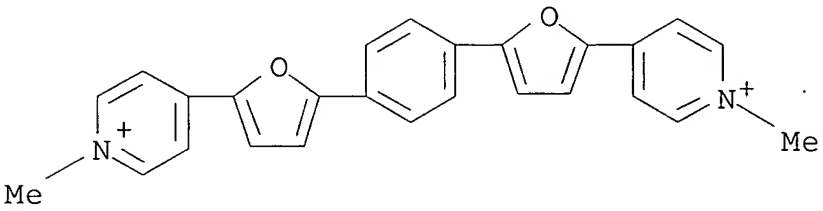
RN 133416-09-8 HCA

CN Pyridinium, 1-methyl-4-[5-[4-[5-(4-pyridinyl)-2-furanyl]phenyl]-2-furanyl]-, iodide (9CI) (CA INDEX NAME)



● I^-

RN 133416-10-1 HCA
CN Pyridinium, 4,4'-(1,4-phenylenedi-5,2-furandiyl)bis[1-methyl-, diiodide (9CI) (CA INDEX NAME)

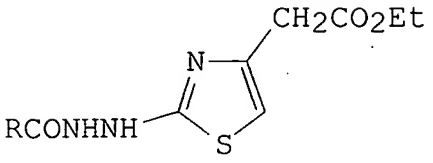


●2 I^-

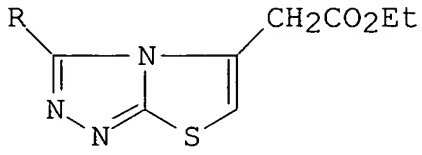
CC 4-3 (Toxicology)
Section cross-reference(s): 14
IT 36913-39-0 101291-08-1 113682-56-7 114254-47-6 133416-06-5 133416-07-6 **133416-08-7 133416-09-8** **133416-10-1** 133416-11-2 133416-12-3 133431-00-2 133431-01-3
(electron transport and respiration by heart and liver mitochondria response to)

L36 ANSWER 25 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 110:75406 HCA
TITLE: Formation of trisubstituted 1,2,4-triazoles in the cyclodehydration of 2-hydrazinothiazoles. Competition of two reaction routes
AUTHOR(S): Veverka, Miroslav; Svetlik, Jan
CORPORATE SOURCE: Inst. Biotechnol., Slovak Tech. Univ., Bratislava, 812 37, Czech.
SOURCE: Liebigs Annalen der Chemie (1989), (1), 75-7

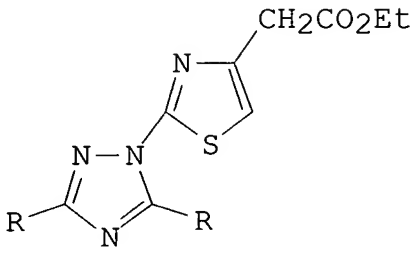
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:75406
GI



I



II



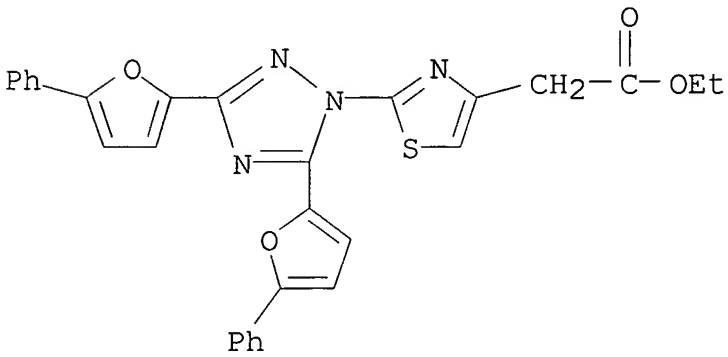
III

AB The intramol. cyclodehydration of Et (2-hydrazinothiazol-4-yl)acetates I (R = Ph, Me, 2-furyl, 5-bromo-2-furyl, 5-phenyl-2-furyl, 2-thienyl) with POCl3 has been re-examined The reactions yield the desired thiazolo[2,3-c]-s-triazoles II together with the unexpected trisubstituted 1,2,4-triazoles III.

IT **117161-71-4P**
(preparation of)

RN 117161-71-4 HCA

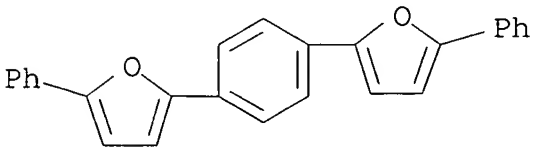
CN 4-Thiazoleacetic acid, 2-[3,5-bis(5-phenyl-2-furanyl)-1H-1,2,4-triazol-1-yl]-, ethyl ester (9CI) (CA INDEX NAME)



CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 66870-62-0P 107366-91-6P 107366-92-7P 107366-97-2P
117161-65-6P 117161-66-7P 117161-67-8P 117161-68-9P
117161-69-0P 117161-70-3P **117161-71-4P** 117161-72-5P
(preparation of)

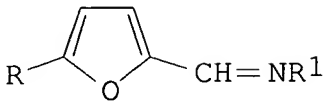
L36 ANSWER 26 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 108:38527 HCA
TITLE: Novel synthesis of heteroaromatic containing electroactive polyaromatics of known linkages, order, topicity and stoichiometry
AUTHOR(S): Pelter, Andrew; Rowlands, Martin; Jenkins, Ieuan H.
CORPORATE SOURCE: Dep. Chem., Univ. Coll. Swansea, Swansea, SA2 8PP, UK
SOURCE: Tetrahedron Letters (1987), 28(43), 5213-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A Pd(0)-catalyzed process for the synthesis of electroactive mixed benzenoid-heteroarom. polymers was given. The polymers had predictable modes of linkage between different units, and the ordering of the units was also fixed. The process could be used for different heterocyclic moieties and for the production of polymers containing the same units, in the same proportions and with the same order but with different topicities.
IT **24387-45-9P**
(preparation of)
RN 24387-45-9 HCA
CN Furan, 2,2'-(1,4-phenylene)bis[5-phenyl- (9CI) (CA INDEX NAME)



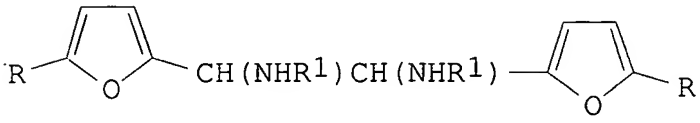
CC 35-7 (Chemistry of Synthetic High Polymers)
IT **24387-45-9P** 112230-46-3P
(preparation of)

L36 ANSWER 27 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 101:110653 HCA
TITLE: Studies in the furan series. XXI. N,N'-Disubstituted difurylethylenediamines. A preparation by hydrodimerization of aldimines
AUTHOR(S): Karaman, B.; Fiser-Jakic, L.; Behluli, M.; Jakopcic, K.

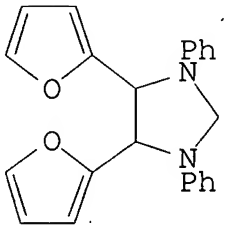
CORPORATE SOURCE: Fac. Technol., Univ. Zagreb, Zagreb, 41000, Yugoslavia
SOURCE: Glasnik Hemicara i Tehnologa Bosne i Hercegovine (1983), Volume Date 1980-1981, 27-28, 81-8
CODEN: GHTBAB; ISSN: 0367-4444
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:110653
GI



I



II

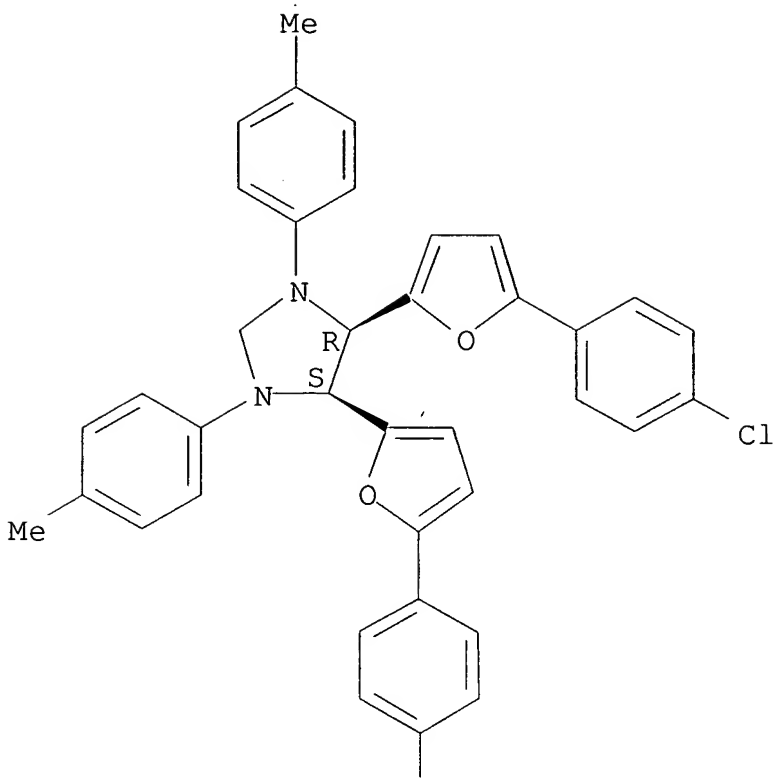


III

AB The reductive dimerization of furfural imines I (R = H, Me, 4-ClC6H4; R1 = Ph, p-tolyl, p-anisyl, PhCH2, cyclohexyl, Bu) by Al gave diamines II. Thus, I (R = H, R1 = Ph) was treated Al/Hg H in ether to give II (R = H, R1 = Ph). The product was treated with HCHO to yield imidazolidine III.
IT **91608-57-0P 91608-58-1P 91608-59-2P**
(preparation of)
RN 91608-57-0 HCA
CN Imidazolidine, 4,5-bis[5-(4-chlorophenyl)-2-furanyl]-1,3-bis(4-methylphenyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



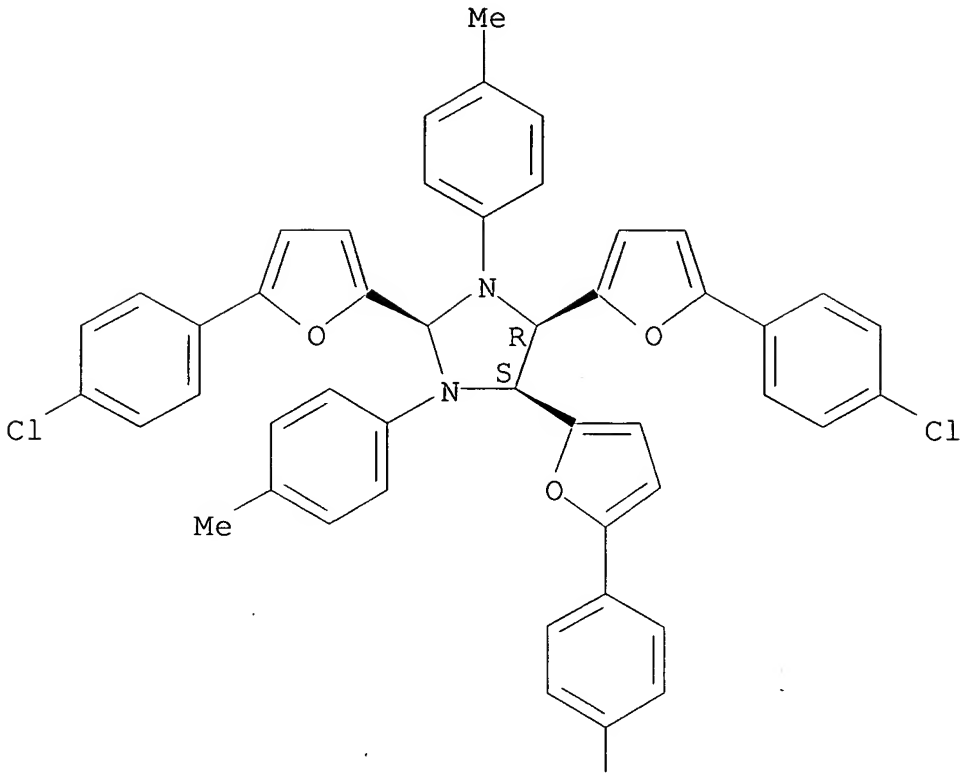
PAGE 2-A

Cl

RN 91608-58-1 HCA
CN Imidazolidine, 2,4,5-tris[5-(4-chlorophenyl)-2-furanyl]-1,3-bis(4-methylphenyl)-, (2α,4α,5α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

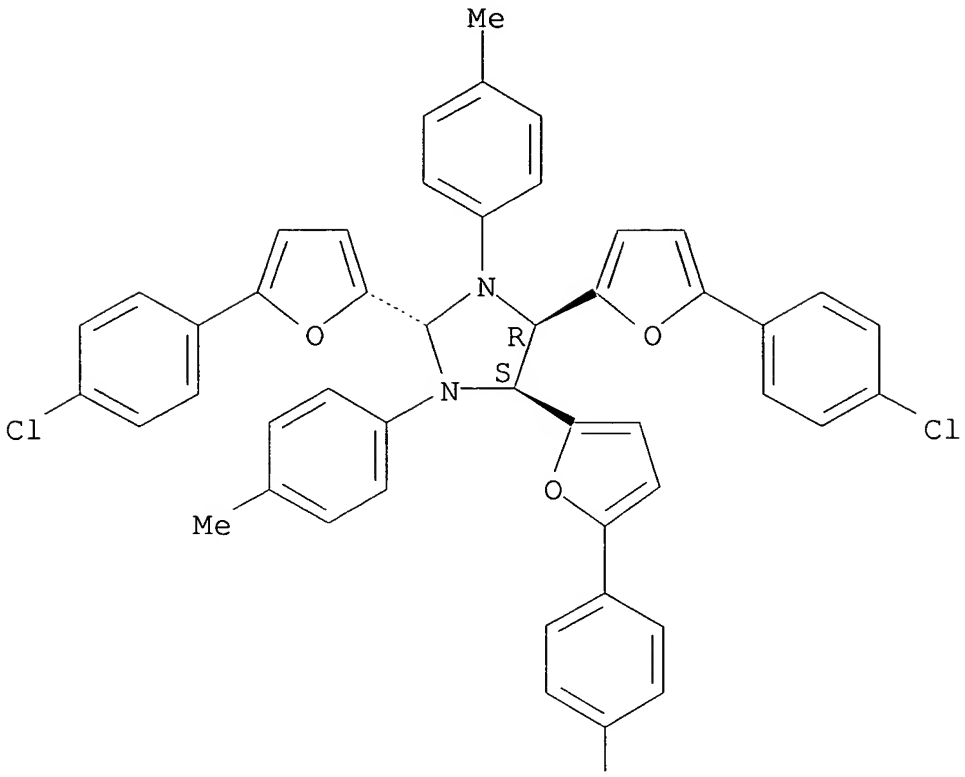


PAGE 2-A

RN 91608-59-2 HCA
CN Imidazolidine, 2,4,5-tris[5-(4-chlorophenyl)-2-furanyl]-1,3-bis(4-methylphenyl)-, (2α,4β,5β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 28

IT 91608-36-5P 91608-37-6P 91608-38-7P 91608-39-8P 91608-40-1P
91608-41-2P 91608-42-3P 91608-43-4P 91608-44-5P 91608-45-6P
91608-46-7P 91608-47-8P 91608-48-9P 91608-49-0P 91608-50-3P
91608-51-4P 91608-52-5P 91608-53-6P 91608-54-7P 91608-55-8P
91608-56-9P **91608-57-0P 91608-58-1P**
91608-59-2P
(preparation of)

L36 ANSWER 28 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 100:51512 HCA

TITLE: Studies on the chemistry of 2-hetarylbenzimidazoles. 5. Acylation of 1-methyl-2-(2'-hetaryl)benzimidazoles

AUTHOR(S): El'chaninov, M. M.; Simonov, A. M.; Oleinikova, L. Ya.

CORPORATE SOURCE: Rostov. Univ., Rostov-on-Don, 344006, USSR

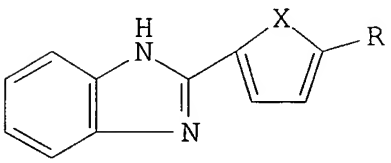
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1983), (10), 1311-13
CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 100:51512

GI



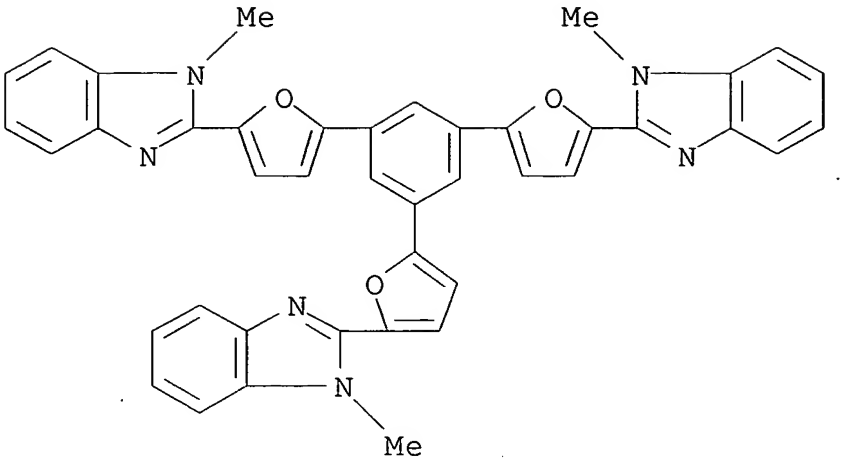
I

AB Formylation of benzimidazoles I (R = H, X = O, S) by urotropine in polyphosphoric acid gave I (R = CHO) in addition to 49% I (R = CH2OH, X = O). Acylation of I (R = H, X = O, S) by R1CO2H (R1 = Me, Ph, o-ClC6H4) gave 22-72% I (R = COR1, X = O, S).

IT **88422-56-4P**
(preparation of)

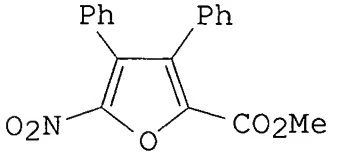
RN 88422-56-4 HCA

CN 1H-Benzimidazole, 2,2',2''-(1,3,5-benzenetriyltri-5,2-furandiyl)tris[1-methyl- (9CI) (CA INDEX NAME)



CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 64480-91-7P 83490-13-5P 83490-14-6P 88422-54-2P 88422-55-3P
88422-56-4P 88422-57-5P 88422-58-6P 88422-59-7P
88422-60-0P
(preparation of)

L36 ANSWER 29 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 94:208623 HCA
TITLE: Synthesis and antimicrobial activity of methyl 5-nitro-3,4-diphenylfuran-2-carboxylate and related compounds
AUTHOR(S): Kuo, Sheng-Chu; Wu, Chun-Hsiung; Huang, Li-Jiau; Yamamoto, Katsumi; Yoshina, Shigetaka
CORPORATE SOURCE: Sch. Pharm., China Med. Coll., Taichung, 400, Taiwan
SOURCE: Chemical & Pharmaceutical Bulletin (1981), 29(3), 635-45
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:208623
GI



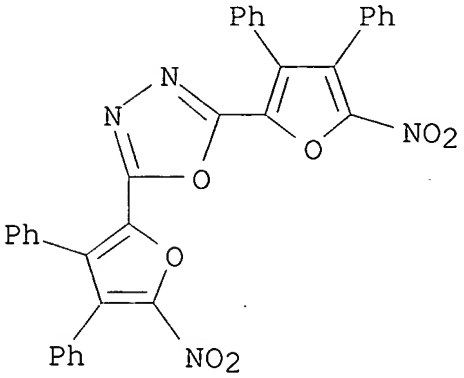
I

AB In order to investigate the antimicrobial activity of derivs. of Me 5-nitro-3,4-diphenylfuran-2-carboxylate (I), the optimal conditions for the nitration of Me 3,4-diphenylfuran-2-carboxylate were studied. Starting from I various amides, hydrazides, hydrazones, oxadiazoles and thiazoles were synthesized and examined for antimicrobial activity. Most of the derivs. were active against Trichomonas vaginalis.

IT **77720-35-5P**
(preparation and antimicrobial activity of)

RN 77720-35-5 HCA

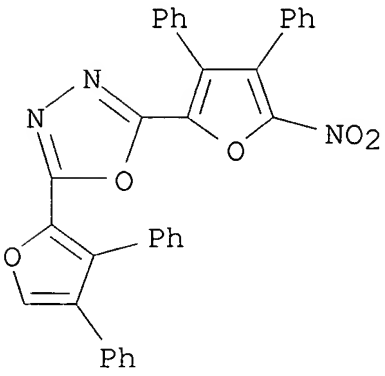
CN 1,3,4-Oxadiazole, 2,5-bis(5-nitro-3,4-diphenyl-2-furanyl)- (9CI) (CA INDEX NAME)



IT **77720-34-4P**
(preparation of)

RN 77720-34-4 HCA

CN 1,3,4-Oxadiazole, 2-(3,4-diphenyl-2-furanyl)-5-(5-nitro-3,4-diphenyl-2-furanyl)- (9CI) (CA INDEX NAME)



CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

IT 52046-98-7P 77719-89-2P 77719-90-5P 77719-91-6P 77719-92-7P
77719-93-8P 77719-94-9P 77719-95-0P 77719-96-1P 77719-99-4P
77720-00-4P 77720-01-5P 77720-02-6P 77720-03-7P 77720-04-8P
77720-05-9P 77720-07-1P 77720-08-2P 77720-12-8P 77720-13-9P
77720-16-2P 77720-17-3P 77720-18-4P 77720-19-5P 77720-20-8P
77720-21-9P **77720-35-5P** 77720-36-6P 77720-37-7P
(preparation and antimicrobial activity of)
IT 52101-39-0P 77719-87-0P 77719-97-2P 77719-98-3P 77720-06-0P
77720-09-3P 77720-10-6P 77720-11-7P 77720-14-0P 77720-15-1P
77720-22-0P 77720-23-1P 77720-24-2P 77720-25-3P 77720-26-4P
77720-27-5P 77720-28-6P 77720-29-7P 77720-30-0P 77720-31-1P
77720-32-2P 77720-33-3P **77720-34-4P** 77720-38-8P
(preparation of)

L36 ANSWER 30 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 84:16976 HCA
TITLE: Dianhydrides of aromatic tetracarboxylic acids
INVENTOR(S): Berlin, A. A.; Liogon'kii, B. I.; Zapadinskii, B. I.
PATENT ASSIGNEE(S): USSR
SOURCE: U.S., 12 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3891633	A	19750624	US 1973-397736	19730917
SU 326862	T	19730810	SU 1970-1386182	19700107
FR 2080900	A5	19711126	FR 1971-329	19710107
FR 2080900	B1	19730608		
PRIORITY APPLN. INFO.:			SU 1970-1386176 A	19700107
			SU 1970-1386177 A	19700107

SU 1970-1386178	A	19700107
SU 1970-1386182	A	19700107
SU 1970-1386186	A	19700107
US 1970-102911	A1	19701230

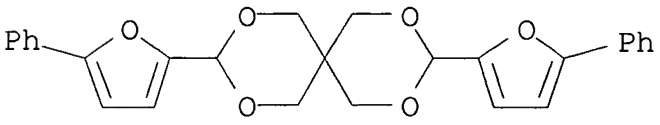
GI For diagram(s), see printed CA Issue.

AB About 20 dianhydrides, e.g. I, II, and III were prepared by Diels-Alder addition of maleic anhydride to furan derivs. followed by cleavage. Thus, p-H2NC6H4NH2 was diazotized and treated with furan and the 1,4-di(α-furyl)benzene cyclized with maleic anhydride to give IV, which was dehydrated with HCl to give I. The anhydrides were useful as monomers.

IT **34121-69-2P 34121-70-5P 34226-51-2P**
(preparation and Diels-Alder reaction with maleic anhydride)

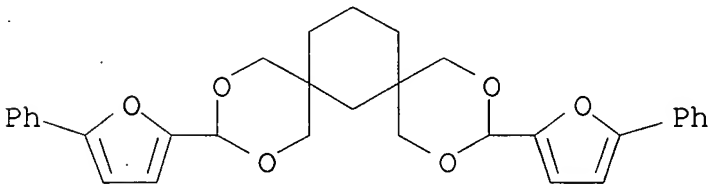
RN 34121-69-2 HCA

CN 2,4,8,10-Tetraoxaspiro[5.5]undecane, 3,9-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



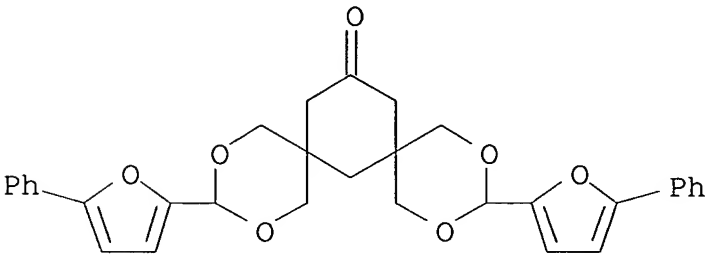
RN 34121-70-5 HCA

CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecane, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



RN 34226-51-2 HCA

CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecan-15-one, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



IC C07C
NCL 260240000G
CC 25-18 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 28, 27, 35
IT 34121-63-6P 34121-64-7P 34121-65-8P 34121-67-0P
34121-69-2P 34121-70-5P 34121-71-6P
34121-72-7P 34178-52-4P 34178-53-5P 34178-54-6P
34226-51-2P 34226-52-3P 52107-55-8P
(preparation and Diels-Alder reaction with maleic anhydride)

L36 ANSWER 31 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 80:95545 HCA
TITLE: Dianhydrides of aromatic tetracarboxylic acids
INVENTOR(S): Berlin, A. A.; Liogon'kii, B. I.; Zapadinskii, B. I.
PATENT ASSIGNEE(S): Institute of Chemical Physics, Academy of Sciences, U.S.S.R.
SOURCE: Brit., 20 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1338932	A	19731128	GB 1971-168	19710101
PRIORITY APPLN. INFO.:			GB 1971-168 A	19710101

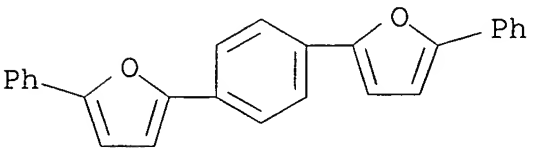
GI For diagram(s), see printed CA Issue.

AB The title anhydrides were prepared by Diels-Alder reaction of maleic anhydride with bis(furyl)arylenes, -tetraoxadispiroalkanes and -alkanones, bis(furfurylidene)diaminoarylenes, and difurfurylarene dicarboxylates followed by dehydration. E.g., 4,4'-bis(α-furyl)diphenyl (I), prepared in 12.6% yield from 4-NH2-(C6H4)2NH2-4.HCl and furan via the 2,5-naphthalenedisulfonic acid diazonium salt, with maleic anhydride gave 77% adduct II which with H2SO4 gave 47% dianhydride (III).

IT **24387-45-9**
(Diels-Alder reaction of, with maleic anhydride)

RN 24387-45-9 HCA

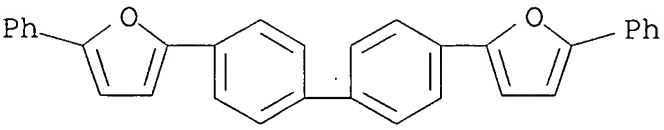
CN Furan, 2,2'-(1,4-phenylene)bis[5-phenyl- (9CI) (CA INDEX NAME)



IT **34121-66-9P 34121-69-2P 34121-70-5P**
34226-51-2P
(preparation of)

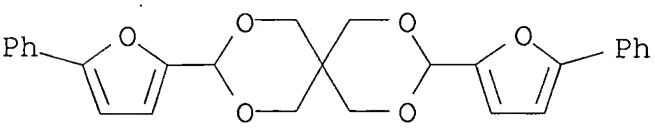
RN 34121-66-9 HCA

CN Furan, 2,2'-[1,1'-biphenyl]-4,4'-diylbis[5-phenyl- (9CI) (CA INDEX NAME)



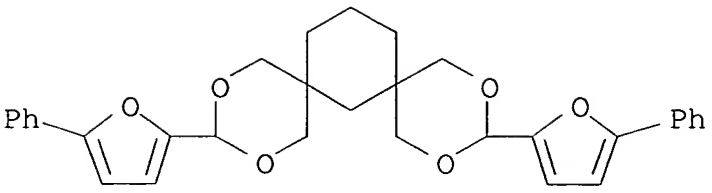
RN 34121-69-2 HCA

CN 2,4,8,10-Tetraoxaspiro[5.5]undecane, 3,9-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)

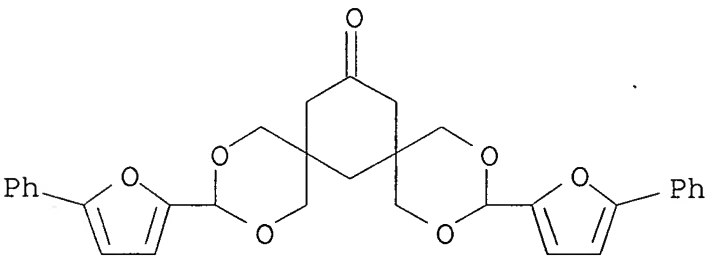


RN 34121-70-5 HCA

CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecane, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



RN 34226-51-2 HCA
CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecan-15-one, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



IC C07C; C07D
CC 25-18 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 27, 28
IT 5115-25-3 **24387-45-9** 26347-56-8 52107-57-0
52107-58-1 52107-59-2 52107-60-5 52107-61-6
(Diels-Alder reaction of, with maleic anhydride)
IT 34119-19-2P 34119-20-5P 34119-21-6P 34119-22-7P 34119-23-8P
34119-24-9P 34119-25-0P 34119-26-1P 34119-27-2P 34119-28-3P
34119-29-4P 34119-30-7P 34119-31-8P 34119-32-9P 34119-33-0P
34119-35-2P 34119-36-3P 34119-37-4P 34119-38-5P 34119-39-6P
34119-40-9P 34119-41-0P 34119-42-1P 34121-63-6P 34121-64-7P
34121-65-8P **34121-66-9P** 34121-67-0P **34121-69-2P**
34121-70-5P 34121-71-6P 34121-72-7P 34121-73-8P
34178-52-4P 34178-53-5P 34178-54-6P **34226-51-2P**
34226-52-3P 34232-41-2P 34232-42-3P 34252-31-8P 34312-00-0P
34560-70-8P 34560-71-9P 48237-13-4P 52107-55-8P 52107-62-7P
52137-88-9P
(preparation of)

L36 ANSWER 32 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 77:114414 HCA
TITLE: α-Arylfuryl derivatives containing spiran groupings
INVENTOR(S): Berlin, A. A.; Liogon'kii, B. I.; Zapadinskii, B. I.

PATENT ASSIGNEE(S): Institute of Chemical Physics, Academy of Sciences, U.S.S.R.
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1972, 49(15), 241. CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

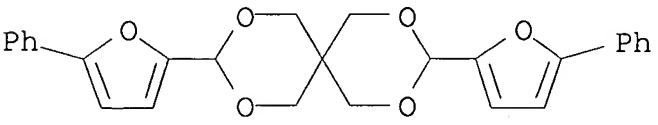
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 303871		19720505	SU	19700107

GI For diagram(s), see printed CA Issue.

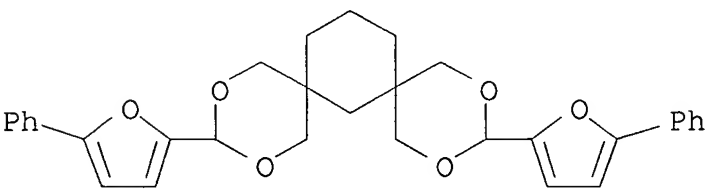
AB The title compds. (I, e.g., R = C, 1,3-cyclohexane-diylidene) or II (R1 = H, OH, O and Z = e.g., phenyl or naphthyl) are produced by treating 5-arylfurfural with pentaerythritol or a tetramethyl derivative of hexane, e.g. 1,1,3,3-tetra-methylolcyclohexane, in the presence of anhydrous ZnCl2.

IT **34121-69-2P 34121-70-5P 38884-02-5P 38886-07-6P**
(preparation of)

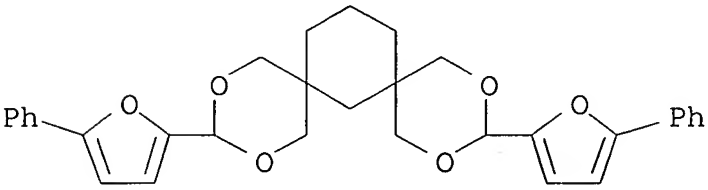
RN 34121-69-2 HCA
CN 2,4,8,10-Tetraoxaspiro[5.5]undecane, 3,9-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



RN 34121-70-5 HCA
CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecane, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)

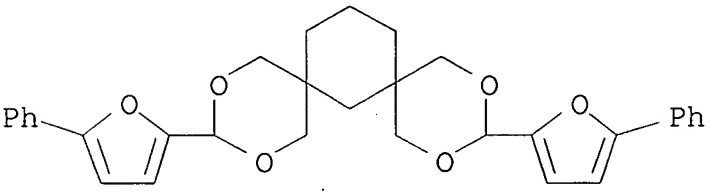


RN 38884-02-5 HCA
CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecanol, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



D1—OH

RN 38886-07-6 HCA
CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecanone, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)

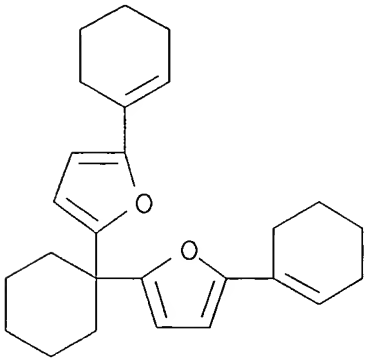


D2═O

IC C07D
CC 28-12 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 25, 26
IT **34121-69-2P 34121-70-5P** 38884-01-4P
38884-02-5P 38884-03-6P 38884-04-7P 38886-06-5P
38886-07-6P
(preparation of)

L36 ANSWER 33 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 76:85630 HCA
TITLE: Condensation of cyclohexanone with furan and pyrrole
AUTHOR(S): Brown, W. H.; Hutchinson, B. J.; MacKinnon, M. H.
CORPORATE SOURCE: Dep. Chem., Univ. Guelph, Guelph, ON, Can.
SOURCE: Canadian Journal of Chemistry (1971), 49(24), 4017-22
CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE: Journal
LANGUAGE: English
AB Several compds. formed by the acid-catalyzed condensation of cyclohexanone with furan and pyrrole were isolated and identified. A previously reported structure for one of the products of the condensation of cyclohexanone with pyrrole was incorrect.
IT **35303-42-5P**
(preparation of)
RN 35303-42-5 HCA
CN Furan, 2,2'-cyclohexylidenebis[5-(1-cyclohexen-1-yl)- (9CI) (CA INDEX NAME)



CC 27 (Heterocyclic Compounds (One Hetero Atom))
IT 35303-40-3P 35303-41-4P **35303-42-5P** 35303-43-6P
35303-44-7P 35303-45-8P 35303-46-9P 35320-70-8P
(preparation of)

L36 ANSWER 34 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 75:151557 HCA
TITLE: Aromatic tetracarboxylic dianhydrides
INVENTOR(S): Berlin, A. A.; Liogon'kii, B. I.; Zapadinskii, B. I.
PATENT ASSIGNEE(S): Institute of Chemical Physics, Academy of Sciences, U.S.S.R.
SOURCE: Ger. Offen., 45 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2100391	A	19710916	DE 1971-2100391	

					197101 07
DE 2100391	B2	19740502			
DE 2100391	C3	19741205			
SU 326862	T	19730810	SU 1970-1386182		
					197001 07
FR 2080900	A5	19711126	FR 1971-329		
					197101 07
FR 2080900	B1	19730608			
PRIORITY APPLN. INFO.:			SU 1970-1386176	A	
					197001 07
			SU 1970-1386177	A	
					197001 07
			SU 1970-1386179	A	
					197001 07
			SU 1970-1386182	A	
					197001 07
			SU 1970-1386186	A	
					197001 07

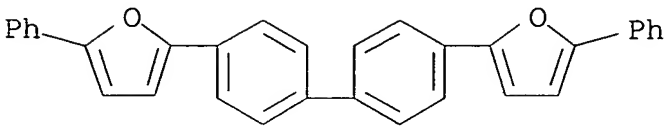
GI For diagram(s), see printed CA Issue.

AB The title compds. [I, R=H, Ph, or naphthyl; X=p-phenylene, (p-C6H4)2CH2, p-(CH:N)2C6H4, p-CH:NC6H4C6H4N:CH-p, (p-C6H4)2O, m- and p-(O2C)2C6H4, and other], useful as crosslinking agents for epoxy and phenol-formaldehyde resins, were prepared by Diels-Alder reaction of bisfurans II with maleic anhydride and dehydration of the adducts (III). Thus, reaction of diazotized p-(H2N)2C6H4 with furan in 5N NaOH for 24 hr gave 10.5% II (R=H, X=p-phenylene), which on reaction with maleic anhydride in THF at 40-60° for 8 hr gave 73% III (R=H, X=p-phenylene) (IV). IV was heated with concentrated HCl in HOAc for 48 hr at 100° to give 62% I (R=H, X=p-phenylene). Similarly prepared were 15 other I.

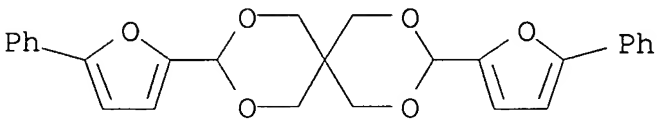
IT **34121-66-9P 34121-69-2P 34121-70-5P 34226-51-2P**
(preparation of)

RN 34121-66-9 HCA

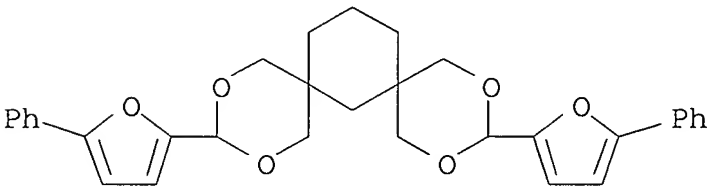
CN Furan, 2,2'-[1,1'-biphenyl]-4,4'-diylbis[5-phenyl- (9CI) (CA INDEX NAME)



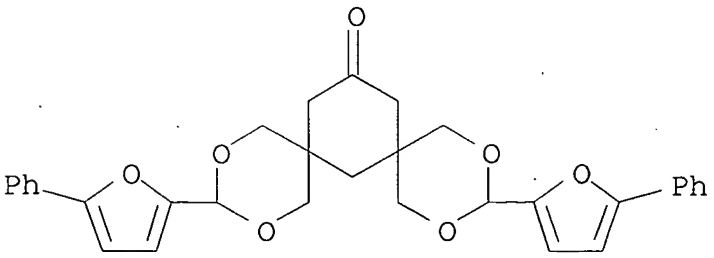
RN 34121-69-2 HCA
CN 2,4,8,10-Tetraoxaspiro[5.5]undecane, 3,9-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



RN 34121-70-5 HCA
CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecane, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



RN 34226-51-2 HCA
CN 2,4,10,12-Tetraoxadispiro[5.1.5.3]hexadecan-15-one, 3,11-bis(5-phenyl-2-furanyl)- (9CI) (CA INDEX NAME)



IC C07BCD; C08G
CC 25 (Noncondensed Aromatic Compounds)
IT 34119-19-2P 34119-20-5P 34119-21-6P 34119-22-7P 34119-23-8P

34119-24-9P 34119-25-0P 34119-26-1P 34119-27-2P 34119-28-3P
34119-29-4P 34119-30-7P 34119-31-8P 34119-32-9P 34119-33-0P
34119-34-1P 34119-35-2P 34119-36-3P 34119-37-4P 34119-38-5P
34119-39-6P 34119-40-9P 34119-41-0P 34119-42-1P 34121-63-6P
34121-64-7P 34121-65-8P **34121-66-9P** 34121-67-0P
34121-68-1P **34121-69-2P** **34121-70-5P**
34121-71-6P 34121-72-7P 34121-73-8P 34178-52-4P 34178-53-5P
34178-54-6P 34178-55-7P **34226-51-2P** 34226-52-3P
34232-41-2P 34232-42-3P 34252-31-8P 34312-01-1P 34560-70-8P
34560-71-9P
(preparation of)

L36 ANSWER 35 OF 35 HCA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 70:24553 HCA
TITLE: Plastic optical elements
INVENTOR(S): Bloom, Stanley M.; Buzzell, Harold O.
PATENT ASSIGNEE(S): International Polaroid Corp.
SOURCE: S. African, 36 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 6705182	A	19680214	ZA 1967-5182	19670831
US 4152332	A	19790501	US 1977-844535	19771025
PRIORITY APPLN. INFO.:			US 1966-577576 A	19660902
			US 1970-60982 A3	19700706
			US 1972-251284 A3	19720508
			US 1974-536419 A3	19741226

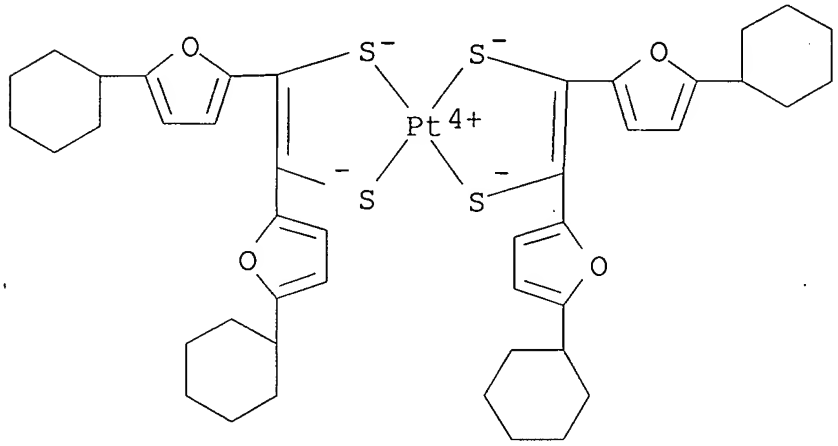
GI For diagram(s), see printed CA Issue.

AB Plastic optical filters like Polaroid glasses are provided with an ir filter layer. The ir absorbing dyestuff is dispersed in a matrix of a cellulose derivative The ir absorbers are metal (Ni, Pd, Pt) complexes of bis[cis-1,2-bis-substituted-1,2-ethylenedithiolate] such as I. Their synthesis has been described by Schrauzer and Mayweg (CA 62: 15738h; 63: 9424f).

IT **23336-27-8**
(in polarizing plastic lenses)

RN 23336-27-8 HCA

CN Platinum, bis[1,2-bis(5-cyclohexyl-2-furyl)-1,2-ethenedithiolato(2-)]- (8CI) (CA INDEX NAME)



CC 73 (Spectra and Other Optical Properties)

IT 14263-04-8 14970-26-4 14977-73-2 15607-55-3 21954-15-4
22920-50-9 22920-51-0 23336-25-6 **23336-27-8**
23408-48-2 23410-72-2 23444-22-6 23725-34-0 23825-57-2
28984-20-5 38951-94-9 38951-96-1 38951-97-2 79404-73-2
(in polarizing plastic lenses)